Electronic Supplementary Information

Life cycle based alternatives assessment (LCAA) for chemical substitution

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S-1 Tiered and life cycle based assessment framework

Respecting the boundary conditions for rapid screening substitution, the proposed *life cycle-based alternatives assessment* (LCAA) framework first identifies the relevant life cycle stages and impacts for all considered chemical-product-function combinations and the relevant attributes to focus higher tiers. These higher tiers are only needed in specific cases. Three tiers are proposed with increasing coverage, from consumer use stage (always needed), to chemical supply chain (needed for evaluating chemical alternatives with fundamentally different supply chains), and up to product life cycle (for evaluating different types of alternatives, e.g. chemicals vs. materials vs. technologies). After initially screening a large number of possible alternatives for the use stage, each tier helps further focusing the number of viable solutions, while avoiding unacceptable trade-offs. For increasing the assessment scope step-by-step, while maintaining an efficient process, we combine indicators from risk assessment and from life cycle impact assessment in line with earlier recommendations.[1] Figure 2 in the main text illustrates the aligned, tiered assessment scope levels. Starting from the relevant chemical functions for a given product application, we define in a pre-screening step the impact categories that might be potentially relevant in the specific application context, advocating for parsimony instead of considering all possible life cycle impacts. Criteria for such considerations are whether the desired chemical function usually requires bioactive chemicals (as in e.g. biocidal agents) or a high weight contribution to a given product (as in e.g. plasticizers). Whereas for the former, toxicity and ecotoxicity impacts are mainly relevant, for the latter, energy-related impacts (climate change, air pollution impacts) are important. Such a strategy is in line with suggestions to select from the wide set of available life cycle impact indicators those that represent the major part of the variation in product life cycle impacts.[2] In addition, any possible alternative that introduces unacceptable trade-offs will be screened out in the pre-screening, such as carcinogens.

After this pre-screening step, the first assessment level (Tier 1) focuses on high-throughput screening of the potential target chemicals and related alternatives. Focus in this step will be on consumer risk and ecosystem impacts related to the product use stage, since direct and usually high exposures are related to this stage. This will identify potential phase-out (i.e. target) chemicals in a given application if not pre-defined, and yield a specific space of alternatives, e.g. for designing new materials or products. Target chemical and suitable candidate alternatives resulting from this high-throughput screening step will at the second level (Tier 2) be compared for emissions and related impacts along the chemical supply chain. Possible trade-offs between, for example, reduced consumer risk and more complex chemical synthesis and related greenhouse gas and air pollutant emissions from increased energy demand will be captured and considered. The remaining, reduced set of suitable candidates is finally compared at the third level (Tier 3) for changes in chemical emissions and related impacts along the full product life cycle, using the product unit function as reference and the impact categories identified in the pre-screening. In this step, additional trade-offs related to, for example, differences in end-of-life handling can be identified and addressed, and remaining suitable candidates ranked.

S-2 Case study followed approach

In the following, we describe for each of the assessment tiers the tier-specific assessment scope, and how the elements of Tables 1−3 in the main text are applied to our case study for establishing inventory flows and impact estimates.

Pre-screening (optional, if target chemical is not known *a priori*)

Inventory analysis – mass of chemical in vinyl flooring: Using a typical vinyl flooring thickness of 3 mm and density of 1500 kg/m^3,[3] the flooring mass per functional unit (i.e. 100

m^2 installed) is 450 kg per average household. Use stage-related chemical inventory data refer to the mass of chemicals in installed flooring product (see Table S4).[4] Since floor maintenance is the same for all vinyl compositions, it is not included in the use phase data. For use stage-related emissions and exposure, we only consider residents of the household where the flooring is installed (i.e. workers installing the flooring are considered as part of supply chain impacts further below. Disposal stage-related emissions are associated with residues in the flooring after 15 years of household use. After product use, the vinyl flooring will be disposed to landfill, where the chemical components can reach the environment (e.g. ambient air, soil and water), which can lead to ecosystem impacts.

Impact assessment: In our product use-related impact pre-screening, we considered consumers (i.e. household residents) exposed to chemicals emitted in the near-field household environment as well as the general population and ecosystems exposed to chemical mass emitted to the far-field outdoor environment during product use and disposal. Fate and exposure are quantified for each flooring constituent using the USEtox-based product intake fraction (PiF) framework linking the chemical mass in flooring to the cumulative intake by users and the general population during use and disposal stages.[4,5] This framework derives chemical transfer fractions during product use from flooring to indoor air (volatilization), surface dust (sorption) and building residents (dust ingestion and dermal contact) and during disposal from landfill to outdoor compartments. We assumed that filler and polymer resin do not migrate out of the flooring, and applied separate models to estimate migration and exposure for semi-volatile substances[6] (DEHP) and for volatile substances[7] (vinyl chloride, finish components), with model input parameters given in Table S4. Transfer to air and dermal exposure for titanium dioxide (inorganic substance) could not be estimated with current models, but only transfer to surface dust (assuming dust concentrations equal initial flooring concentrations) and related ingestion exposure was considered, acknowledging that overall exposure is underestimated. Due to unclear physicochemical properties, toxicity impacts could not be estimated for epoxidized fish oil fatty acids (unclear physiochemical properties). Chemical transfer from landfill to outdoor air, water, and soil during disposal is estimated using the MOCLA model.[8] Transfer fractions from flooring and landfill are combined to obtain cumulative exposure (product intake fractions, PiF) of residents and the general population.[5] According to Table 1 (main text), PiF exposure estimates are multiplied by the initial substance mass in flooring to yield exposure doses. Combining these doses with cancer slope factors and reference doses respectively yields cancer risk and hazard quotient estimates. Cumulative chemical transfer fractions from flooring to freshwater are combined with initial mass in flooring and ecotoxicity effect information to yield ecotoxicity impact scores.

Tier 1: Selection and screening of possible alternatives based on use stage impacts

Possible functionally equivalent chemical alternatives to DEHP plasticizer in the given product use context have been identified from the Pharos database and the literature to be screened for use stage related impacts (Tier 1).[9-11] Identified possible alternatives and their physiochemical properties are given in Table S3.

Inventory analysis: To maintain equal functional performance, flooring weight fractions of alternative plasticizers as compared to DEHP have been adjusted using a substitution factor relating material hardness properties of alternatives to those of DEHP. Substitution factors for all listed possible alternatives are ≤ 1 (i.e. equal or slightly better hardness performance compared to DEHP; see Table S3). The same approach is applied to the possible alternatives as described above in the pre-screening step.

Impact assessment: We screened the identified possible alternatives against DEHP for exposure and hazard associated with the use stage of the flooring product following the approach described in the previous section.

Tier 2: Comparison of supply chain impacts for selected plasticizer alternatives

As starting point for evaluating chemical supply chain impacts, the required manufactured flooring mass per functional unit amounts to 493 kg in order to yield 450 kg installed flooring per average household, since 4.5% of vinyl flooring material is on average sent to landfill as manufacturing waste,[12] and additionally about 4.5% is cut off later as installation waste.[13] The resulting mass of flooring waste is therefore 43 kg.

Inventory analysis: Chemical supply chain emissions of hundreds of chemicals from industrial processes, energy conversion and transport for producing the target chemical and its two alternative selected plasticizers were derived from the Environmental Genome of Industrial Processes (EGIP).[14] In EGIP, a detailed analysis of the chemical processing is performed to determine the mass of reactants needed to produce the target chemical (or its alternative) at the necessary purity, and provide related amounts of environmental emissions at every step (see Section S-8 for details).[15] The emissions include chemical process emissions and the chemicals from the production of the array of energy (steam, electricity, furnaces, etc.) used in these chemical manufacturing processes. The flows represented in an EGIP dataset are illustrated in Fig. 5 (main text) for DEHP as example chemical, with additional details given for DEHP and the two selected alternatives in Section S-8.

Impact assessment: Chemical supply chain emissions were characterized in terms of impacts on human health, ecosystem quality, and climate change by combining chemical-specific emissions with respective characterization factors expressed as potential impacts per unit emission (Table 2, main text). To arrive at total plasticizer supply chain related climate change impacts, we used IPCC global warming potentials (GWP),[16] expressed in kg CO_2-equivalents per kg chemical emitted, summed over all chemicals. For toxicity-related impacts on human health and on ecosystem quality, the chemical-specific mass emitted to air (equally assigned to urban and rural air), freshwater and natural soil are characterized in terms of cancer and non-cancer population-level potential lifetime loss (humans) and potential species loss (ecosystems) using the scientific consensus model USEtox,[17] which is widely used in comparative assessments.[18,19] Species loss is expressed as potentially disappeared fraction (PDF) of ecosystem species exposed over a given time and freshwater volume per unit mass emitted, commonly applied in comparative assessments for damages on ecosystem quality.[20,21] Human lifetime loss is expressed as disability-adjusted life years (DALY), commonly applied as comparative measure for population-level health impacts.[22] For impacts from exposure to air pollutants, we use fine particulate matter ($PM_{2.5}$) as most consistent and robust predictor of adverse health effects in long-term air pollution exposure studies.[23,24] Related human health impacts are obtained by multiplying emissions with recommended characterization factors expressed in DALY per kg $PM_{2.5}$ or precursor (i.e. NH_3, NO_x, and SO_2) using average effect factors,[21] based on consistent information for population exposure[25] and exposure-response slopes.[26] While flooring installation-related impacts are already included in the use stage evaluation for adult users (mostly relevant for volatile flooring constituents), workers might be exposed to chemicals used in the various manufacturing steps along the chemical supply chain. We evaluated toxicity-related impacts on workers for the plasticizer supply chain by using an input-output matrix-based approach[27] to first determine as inventory flow the number of blue collar worker hours in each manufacturing sector of the U.S. economy for the economic value spent for the plasticizer in the plasticizer manufacturing sector (North American Industry Classification System (NAICS) code: 325199), i.e. for an average costs of 1 USD for purchasing 1 kg plasticizer.[28] The total worker impacts per functional unit due to workplace inhalation exposure in the entire chemical supply chain are obtained by multiplying the blue collar hours worked in each sector by characterization factors, expressed in DALY per blue collar worker hour in each sector. These characterization factors were calculated as the product of worker standard breathing rate, sector-specific average measured concentrations from 235 commonly applied industrial substances and chemical-specific cancer and non-cancer dose-responses.[29]

Tier 3: Vinyl flooring material life cycle impacts

Inventory analysis: Inventory information on emissions from industrial processes, energy conversion and transport to air, water, and soil over the entire life cycle of the vinyl flooring are derived from EGIP[14] for the selected alternative plasticizers and all relevant flooring constituents (see Table S4). For waste, we included emissions associated with manufacturing and installation waste, which refers to the 43 kg of flooring waste that is produced per functional unit, as well as the emissions due to the landfilling of the entire flooring material after use, obtained from ecoinvent[30] or calculated with the MOCLA landfill model.[8] The full inventory data are given in Section S-10.

Impact assessment: In addition to use stage and chemical supply chain impacts from three plasticizer alternatives, life cycle impacts on climate change, human health and ecosystem quality for all other vinyl flooring constituents were calculated following the same approach as for chemical supply chain impacts (Table 3, main text). Toxicity-related worker impacts in the sector producing the vinyl flooring (i.e. laminated plastics plate, sheet except packaging, and shape manufacturing, NAICS code: 326113) were assessed following the approach detailed for chemical supply chain worker impacts, and using average costs of 7 USD/m^2 vinyl flooring.[31] Life cycle worker impacts thereby include plasticizer manufacturing impacts on workers from Tier 2. To evaluate the contribution of climate change impacts on human health as compared to toxicity and $PM_{2.5}$-related impacts, climate change impacts were also translated into DALY/kg emitted.[32]

S-3 Case study vinyl flooring composition data

As common building material, we selected vinyl flooring reported to be among the major indoor emission sources of phthalate plasticizers.[33,34] We constructed the chemical composition of a homogeneous, single layer vinyl flooring based on the environmental product declarations (EPD) of two commercial flooring products,[12,13] and information from the Pharos database.[9] The chemical composition of the case study flooring material is provided in Table S1.

Table S1. Chemical composition of 450 kg of homogeneous, single layer 3 mm vinyl flooring material installed in a 100 m^2 average household.

Chemical function in flooring material	Chemical constituent	CAS RN	Mass fraction (%)	Mass in household flooring (kg)
Filler	Calcium carbonate ($CaCO_3$)	471-34-1	41.9	188.6
Resin polymer	Polyvinyl chloride (PVC)	9002-86-2	36.564	164.5
Monomer residues	Vinyl chloride monomer (VCM)	75-01-4	0.036[a]	0.16
Plasticizer	di(2-ethylhexyl) phthalate (DEHP)	117-81-7	15.6	70.2
Stabilizer	Fatty acids, C14-22, 2-ethylhexyl esters, epoxidized	95370-96-0	4.4	19.8
Pigment	Titanium dioxide (TiO_2)	13463-67-7	0.5	2.25
Finish	*Sum of finish constituents*		1.0	4.5
	Aromatic naphtha, type 1	64742-95-6	0.03	0.14
	Ethylbenzene (C_8H_{10})	100-41-4	0.01	0.05
	1,2,4-trimethylbenzene (C_9H_{12})	95-63-6	0.02	0.09
	Diethylene glycol diethyl ether ($C_8H_{18}O_3$)	112-36-7	0.94	4.23

[a] Monomer residues range from 1 to 1000 ppm of PVC, of which we assumed the worst-case (1000 ppm of PVC) to be residues in vinyl flooring.

S-4 Case study physicochemical substance properties

Table S2 and Table S3 provide substance properties for all case study plasticizers.

Table S2 Physiochemical properties of DEHP used as plasticizer in vinyl flooring.

Parameter	DEHP
CAS RN	117-81-7
Molecular weight, *MW* (g/mol)[35]	390.57
Vapor pressure, P_v (Pa)[35]	5.03×10^{-5}
Partition coefficient between octanol and water, log K_{ow} (–)[35]	7.6
Partition coefficient between octanol and air, log K_{oa} (–)[35]	13.31
Diffusion coefficient in vinyl flooring, D_m (m^2/s)[36]	1.22×10^{-13}
Partition coefficient between vinyl flooring and air, K_{ma} (–)[37]	1.98×10^{10}
Partition coefficient between vinyl flooring and water, K_{mw} (–)[38]	6.87×10^{6}

Parameter	DEHP
Diffusion coefficient in sorption material (gypsum board), D_s (m^2/s)[(36)]	1.23×10^{-12}
Partition coefficient between sorption material and air, K_s (−)[(37)]	4.44×10^{9}
Initial concentration in vinyl flooring, C_0 (μg/m^3)[(*)]	2.34×10^{11}
Initial mass in 100 m^2 vinyl flooring, m_0 (kg)[(**)]	70.2

*Calculated from the mass, thickness, area and plasticizer weight fraction in vinyl flooring per functional unit. **Calculated from C_0 and 450 kg of installed flooring for a 100 m^2 household.

Table S3. Physiochemical properties of possible alternatives* to DEHP as plasticizer used in vinyl flooring. Parameter symbols, units and sources are given in Table S2.

Parameter	DIHP	BBP	DBP	DEHA	97A	DBS	TXIB	ATBC	DEHAP
CAS RN	71888-89-6	85-68-7	84-74-2	103-23-1	68515-75-3	109-43-3	6846-50-0	77-90-7	298-07-7
SF**	0.97[(39)]	0.94[(39)]	0.86[(39)]	0.93[(39)]	~1[(39)]	0.72[(40)]	~1[(41)]	~1[(41)]	1.0[(10)]
MW	362.51	312.36	278.34	370.57	356.55	314.46	286.41	402.48	322.42
P_v	1.1×10^{-3}	5.2×10^{-4}	4.2×10^{-3}	1.5×10^{-4}	8.9×10^{-3}	7.2×10^{-4}	6.4×10^{-1}	1.4×10^{-4}	2.4×10^{-3}
$\log K_{ow}$	7.41	3.81	4.41	6.86	7.55	5.97	4.8	2.15	−1.86
$\log K_{oa}$	10.97	7.9	7.6	11.65	10.35	10.98	10.16	8.07	2.83
D_m	1.5×10^{-13}	2.1×10^{-13}	2.8×10^{-13}	1.4×10^{-13}	1.5×10^{-13}	2.1×10^{-13}	2.6×10^{-12}	1.1×10^{-13}	2×10^{-13}
K_{ma}	5.4×10^{8}	4.7×10^{6}	3×10^{6}	1.5×10^{9}	2.1×10^{8}	5.4×10^{8}	1.5×10^{8}	6.2×10^{6}	1.9×10^{3}
K_{mw}	4.2×10^{6}	2.9×10^{2}	1.4×10^{3}	9.5×10^{5}	6.1×10^{6}	8.9×10^{4}	4×10^{3}	3.4	7.9×10^{-5}
D_s	1.5×10^{-12}	2.2×10^{-12}	2.9×10^{-12}	1.4×10^{-12}	1.6×10^{-12}	2.1×10^{-12}	2.7×10^{-12}	1.1×10^{-12}	2×10^{-12}
K_s	1.2×10^{8}	1.1×10^{6}	6.6×10^{5}	3.4×10^{8}	4.6×10^{7}	1.2×10^{8}	3.4×10^{7}	1.4×10^{6}	4.2×10^{2}
m_0	68.09	65.99	60.37	65.29	70.2	50.54	70.2	70.2	70.2

*DIHP: di(isoheptyl)phthalate; BBP: butyl benzyl phthalate; DBP: dibutyl phthalate; DEHA: di(ethylhexyl) adipate; 97A: di-C7-9-branched and linear alkyl esters; DBS: dibutyl sebacate; TXIB: butane ester 2,2,4-trimethyl 1,3-pentanediol diisobutyrate; ATBC: o-acetyl tributyl citrate; DEHAP: di(2-ethylhexyl) phosphate. **Substitution factor: calculated as ratio of weight fraction of substance vs. weight fraction of DEHP for providing equal material hardness properties under room conditions.[39]

S-5 Case study product use stage input data

Table S4 contains case study input data for calculating product use related chemical transfer fractions from vinyl flooring as basis for exposure, risk and impact estimates.

Table S4. Input data for calculating use-stage chemical transfer fractions from vinyl flooring.

Parameter	Value
Household volume (m^3)[(42,*)]	236
Room air exchange rate (h^{-1})[(42,*)]	0.79

Parameter	Value
Flooring area in entire household (m^2)[42,43,**]	113.6
Area of other indoor sorption surfaces in entire household (m^2)[42,44,45,***]	587.2
Flooring use duration (d)[****]	5475
Number of adult occupants in household (capita)[****]	2
Number of child occupants under 5 years old in household (capita)[****]	1
Body weight of adult (kg)[34]	80
Body weight of child (kg)[34]	13.8
Dust ingestion rate per adult (mg/d)[7]	60
Dust ingestion rate per child (mg/d)[7]	59.34
Inhalation rate per adult (m^3/d)[34]	16
Inhalation rate per child (m^3/d)[34]	8.9

*OECD countries average was used as reference. **Volume of North American households of 277 m^3 [42] multiplied by a carpet area per household of 0.41 m^2/m^3 [43]. ***Volume of North American households of 277 m^3 [42] multiplied by the total surface area per household of 2.53 m^2/m^3 [44,45] minus the flooring area per household of 113.6 m^2. ****Own assumption.

S-6 Product use related risks and ecosystem impacts of vinyl flooring

Table S5 and Table S6 respectively contain case study results for product use related human health risks and ecosystem impacts of all chemical constituents considered in a typical vinyl flooring material.

Table S5. Product use related product intake fractions,[a] reference doses,[b] cancer slope factors,[b] and derived non-cancer hazard quotients[c] and cancer risk probability[c] for chemical constituents in 100 m^2 vinyl flooring. VCM: vinyl chloride monomer, TiO_2: titanium dioxide, C_8H_{10}: ethylbenzene, C_9H_{12}: 1,2,4-trimethylbenzene, $C_8H_{18}O_3$: diethylene glycol diethyl ether.

Parameter	Plasticizer	Monomer	Stabilizer	Pigment	Finish			
	DEHP	VCM	Fatty acids	TiO_2	Naphtha	C_8H_{10}	C_9H_{12}	$C_8H_{18}O_3$
CAS RN	117-81-7	75-01-4	95370-96-0	13463-67-7	64742-95-6	100-41-4	95-63-6	112-36-7
PiF: product intake fraction [−]								
User-child inhalation	2.6E-05	2.0E-03	2.0E-03	n/a	2.0E-03	2.0E-03	2.0E-03	2.0E-03
User-child ingestion	3.6E-04	3.6E-09	1.4E-07	6.4E-04	6.5E-07	5.8E-08	4.7E-08	1.2E-08
User-child dermal	3.8E-06	2.8E-06	2.1E-04	n/a	5.9E-05	3.9E-06	3.7E-06	5.1E-06
User-adult inhalation	9.2E-05	7.1E-03	7.1E-03	n/a	7.1E-03	7.1E-03	7.1E-03	7.1E-03
User-adult ingestion	6.1E-04	6.0E-09	2.4E-07	1.3E-03	1.1E-06	9.8E-08	7.9E-08	2.1E-08
User-adult dermal	6.7E-06	6.9E-07	1.3E-03	n/a	2.5E-04	7.7E-06	5.9E-06	1.8E-06
Population inhalation	1.7E-07	1.4E-05	1.4E-05	n/a	1.2E-05	8.7E-06	7.0E-06	1.2E-05
Population ingestion	2.8E-06	1.2E-09	2.4E-05	n/a	1.7E-07	7.2E-10	4.3E-10	1.5E-08
Population dermal	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
RfD: reference dose [mg/(kg/d)]								
Inhalation	2.8E-02	1.0E-01	n/a	2.8E-03	1.0E-01	1.0E+00	7.0E-03	5.0E-02
Ingestion	2.0E-02	3.0E-03	n/a	2.3E+00	3.0E-02	1.0E-01	4.0E-02	7.3E+00
Dermal	3.8E-03	3.0E-03	n/a	2.3E+00	1.8E+00	9.7E-02	4.0E-02	4.9E+00
CSF: cancer slope factor [(mg/(kg/d))$^{-1}$]								
Inhalation	5.2E-03	3.5E-01	n/a	n/a	n/a	4.2E-02	4.7E-04	n/a
Ingestion	5.2E-03	2.7E-01	n/a	n/a	n/a	4.7E-04	4.7E-04	n/a
Dermal	7.4E-02	2.7E-01	n/a	n/a	n/a	4.7E-04	4.7E-04	n/a
HQ: hazard quotient [−]								
User-child	1.9E+01	4.5E-02	n/a	8.1E-03	3.5E-02	1.2E-03	3.4E-01	2.2E+00
User-adult	2.9E+00	1.3E-02	n/a	1.4E-03	1.1E-02	3.7E-04	1.0E-01	6.8E-01
Population	2.3E-11	5.1E-14	n/a	n/a	3.9E-14	8.9E-16	2.1E-13	2.3E-12
R: cancer risk [−]								
User-child	2.2E-03	1.5E-03	n/a	n/a	n/a	5.0E-05	1.1E-06	n/a
User-adult	3.3E-04	4.6E-04	n/a	n/a	n/a	1.5E-05	3.4E-07	n/a
Population	2.5E-15	1.8E-15	n/a	n/a	n/a	3.8E-17	6.8E-19	n/a

[(a)] Product intake fractions are derived with the PiF modeling framework using the "article interior" module.[5] Scenario input data are given in Table S4.

[(b)] Reference doses and cancer slope factors are determined based on reported test data as provided in different sources, including USEtox,[17] US EPA's Integrated Risk Information System (IRIS),[46] Provisional Peer-Reviewed Toxicity Values (PPRTV),[47] US EPA's Chemistry Dashboard,[48] and the Carcinogenic Potency Database (CPDB).[49] Where data for inhalation or dermal exposure were missing, we applied 1:1 route-to-route extrapolation from ingestion data or used a QSAR model.[50] Where reference concentrations for inhalation were available, they were first converted to doses.

[(c)] Non-cancer hazard quotients and cancer risks are based on intake doses, which were derived from product intake fractions according to Table 1 (main text).

Table S6. Product use related cumulative chemical transfer fractions,[(a)] chemical fractions sent to landfill,[(a)] bulk removal rate constants,[(a)] bioavailable chemical mass fractions,[(b)] hazard concentrations,[(c)] and derived ecotoxicity impact scores[(d)] for chemical constituents in 100 m^2 vinyl flooring. VCM: vinyl chloride monomer, TiO_2: titanium dioxide, C_8H_{10}: ethylbenzene, C_9H_{12}: 1,2,4-trimethylbenzene, $C_8H_{18}O_3$: diethylene glycol diethyl ether.

Parameter	**Plasticizer**	**Monomer**	**Stabilizer**	**Pigment**	**Finish**			
	DEHP	VCM	Fatty acids	TiO_2	Naphtha	C_8H_{10}	C_9H_{12}	$C_8H_{18}O_3$
CAS RN	117-81-7	75-01-4	95370-96-0	13463-67-7	64742-95-6	100-41-4	95-63-6	112-36-7
Tcum: cumulative chemical transfer fraction [–]								
Freshwater	2.2E-02	7.1E-05	4.0E-02	n/a	6.8E-04	7.6E-06	9.1E-06	8.7E-04
f_{SWT}: fraction of chemical sent to solid waste treatment (SWT) after product use [–]								
Landfill	9.9E-01	n/a	n/a	n/a	n/a	n/a	n/a	n/a
k_{loss}: bulk removal rate constant [d^{-1}]								
Freshwater	5.5E-02	2.8E-01	6.5E-02	n/a	1.9E-01	2.5E-01	2.1E-01	2.0E-01
XF: bioavailable (i.e. truly dissolved) chemical fraction [–]								
Freshwater	7.3E-02	1.0E+00	1.0E+00	7.3E-02	1.0E+00	1.0E+00	1.0E+00	1.0E+00
HC50: hazard concentration affecting 50% of exposed species [mg/L]								
Freshwater	2.0E-02	3.2E+02	4.0E+01	1.9E+01	1.0E+01	3.3E+00	2.8E+00	4.1E+03
ETS: ecotoxicity impact scores [PDF m^3 d]								
Freshwater	2.5E+04	3.3E-05	9.4E+01	n/a	5.9E-01	9.5E-03	2.7E-01	7.5E-02

[(a)] Cumulative chemical transfer fractions, fractions sent to landfill after product use, and bulk removal rate constants in (continental) freshwater are derived with the PiF modeling framework using the “article interior” module.[5]

[(b)] Bioavailable chemical mass fractions in (continental) freshwater are derived with USEtox.[17]

[(c)] Hazard concentrations, yielding the same level are determined based on reported test data as provided in different sources, including USEtox[17] and US EPA’s Chemistry Dashboard,[48] or were estimated using a machine learning model.[51] While generally, we recommend deriving effect factors from 0.2/HC20 (see Table 1, main text) in line with current recommendations,[52] we used in our case study 0.5/HC50 as proxy until the HC20-based approach is implemented for the wide range of relevant chemicals.

[(d)] Ecotoxicity impact scores were derived according to Table 1 (main text).

S-7 Product use related risks and ecosystem impacts of plasticizers

Table S7 and Table S8 respectively contain case study results for product use related human health risks and ecosystem impacts of all considered plasticizer alternatives (see Table S3) in a typical vinyl flooring material, with related single scores for each impact type provided in Figure S1.

Table S7. Product use related product intake fractions,[(a)] reference doses,[(b)] cancer slope factors,[(b)] and derived non-cancer hazard quotients[(c)] and cancer risk probability[(c)] for considered alternative plasticizers in 100 m^2 vinyl flooring.

Parameter	Phthalate				Adipate		Dioate	Butyrate	Citrate	Phosphate
	DEHP	DIHP	BBP	DBP	DEHA	97A	DBS	TXIB	ATBC	DEHPA
CAS RN	117-81-7	71888-89-6	85-68-7	84-74-2	103-23-1	68515-75-3	109-43-3	6846-50-0	77-90-7	298-07-7
PiF: product intake fraction [–]										
User-child inhalation	2.6E-05	3.5E-05	1.7E-03	1.9E-03	2.8E-05	6.8E-05	3.5E-05	8.8E-05	1.5E-03	1.9E-03
User-child ingestion	3.6E-04	3.0E-04	4.5E-05	3.0E-05	3.4E-04	2.3E-04	3.0E-04	2.1E-04	5.4E-05	3.0E-08
User-child dermal	3.8E-06	1.2E-04	1.1E-03	7.4E-04	4.7E-05	2.3E-04	1.6E-04	6.2E-04	1.1E-03	2.9E-03
User-adult inhalation	9.2E-05	1.3E-04	6.2E-03	6.9E-03	1.0E-04	2.4E-04	1.3E-04	3.2E-04	5.5E-03	6.9E-03
User-adult ingestion	6.1E-04	5.0E-04	7.5E-05	5.1E-05	5.7E-04	4.0E-04	5.0E-04	3.6E-04	9.1E-05	5.1E-08
User-adult dermal	6.7E-06	7.4E-04	6.9E-03	4.7E-03	2.6E-04	1.5E-03	8.3E-04	3.2E-03	6.5E-03	1.8E-02
Population inhalation	1.7E-07	2.2E-07	9.6E-06	1.0E-05	1.8E-07	4.4E-07	2.2E-07	5.3E-07	9.3E-06	1.1E-05
Population ingestion	2.8E-06	3.9E-06	2.6E-05	1.7E-05	2.9E-06	5.4E-06	3.0E-06	1.3E-05	5.2E-05	7.7E-05
Population dermal	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
RfD: reference dose [mg/(kg/d)]										
Inhalation	2.8E-02	1.8E+00	1.2E-01	2.8E-01	6.0E-01	9.8E+00	2.4E+00	3.0E+00	7.3E-01	6.1E+00
Ingestion	2.0E-02	1.8E+00	2.0E-01	1.0E-01	6.0E-01	9.8E+00	2.4E+00	1.8E+00	7.3E-01	6.1E+00
Dermal	3.8E-03	1.8E+00	1.2E-01	1.0E-01	4.9E+00	9.8E+00	2.4E+00	1.8E+00	7.3E-01	6.1E+00
CSF: cancer slope factor [(mg/(kg/d))$^{-1}$]										
Inhalation	5.2E-03	n/a	2.0E-03	n/a	9.4E-04	n/a	n/a	n/a	n/a	n/a
Ingestion	5.2E-03	n/a	2.0E-03	n/a	9.4E-04	n/a	n/a	n/a	n/a	n/a
Dermal	7.4E-02	n/a	3.1E-03	n/a	9.4E-04	n/a	n/a	n/a	n/a	n/a
HQ: hazard quotient [–]										
User-child	1.9E+01	2.2E-01	2.1E+01	1.2E+01	5.4E-01	5.0E-02	1.4E-01	4.5E-01	3.4E+00	7.4E-01
User-adult	2.9E+00	5.8E-02	8.2E+00	4.9E+00	8.7E-02	1.7E-02	3.5E-02	1.6E-01	1.3E+00	3.3E-01
Population	2.3E-11	3.5E-13	3.1E-11	2.8E-11	7.6E-13	9.7E-14	1.5E-13	1.2E-12	1.3E-11	2.3E-12
R: cancer risk [–]										
User-child	2.2E-03	n/a	6.0E-03	n/a	3.4E-04	n/a	n/a	n/a	n/a	n/a
User-adult	3.3E-04	n/a	2.6E-03	n/a	6.5E-05	n/a	n/a	n/a	n/a	n/a
Population	2.5E-15	n/a	1.0E-14	n/a	4.3E-16	n/a	n/a	n/a	n/a	n/a

[(a)] Product intake fractions are derived with the PiF modeling framework using the "article interior" module.[5] Scenario input data are given in Table S4.

[(b)] Reference doses and cancer slope factors are determined based on reported test data as provided in different sources, including USEtox,[17] US EPA's Integrated Risk Information System (IRIS),[46] Provisional Peer-Reviewed Toxicity Values (PPRTV),[47] US EPA's Chemistry Dashboard,[48] and the Carcinogenic Potency Database (CPDB).[49] Where data for inhalation or dermal exposure were missing, we applied 1:1 route-to-route extrapolation from ingestion data or used a QSAR model.[50] Where reference concentrations for inhalation were available, they were first converted to doses.

[(c)] Non-cancer hazard quotients and cancer risks are based on intake doses, which were derived from product intake fractions according to Table 1 (main text).

Table S8. Product use related cumulative chemical transfer fractions,[(a)] chemical fractions sent to landfill,[(a)] bulk removal rate constants,[(a)] bioavailable chemical mass fractions,[(b)] hazard concentrations,[(c)] and derived ecotoxicity impact scores[(d)] for considered alternative plasticizers in 100 m^2 vinyl flooring.

Parameter	Phthalate				Adipate		Dioate	Butyrate	Citrate	Phosphate
	DEHP	DIHP	BBP	DBP	DEHA	97A	DBS	TXIB	ATBC	DEHPA
CAS RN	117-81-7	71888-89-6	85-68-7	84-74-2	103-23-1	68515-75-3	109-43-3	6846-50-0	77-90-7	298-07-7
Tcum: cumulative chemical transfer fraction [–]										
Freshwater	2.2E-02	3.2E-02	1.2E-02	1.2E-02	3.4E-02	2.6E-02	3.7E-02	6.1E-02	1.1E-01	3.5E-02
f_{SWT}: fraction of chemical sent to solid waste treatment (SWT) after product use [–]										
Landfill	9.9E-01	9.8E-01	1.1E-01	2.2E-02	9.8E-01	9.6E-01	9.8E-01	9.5E-01	2.1E-01	7.5E-12
k_{loss}: bulk removal rate constant [d^{-1}]										
Freshwater	5.5E-02	2.8E-02	6.0E-02	1.2E-01	8.9E-02	3.0E-02	9.0E-02	2.6E-02	8.8E-02	5.3E-02
XF: bioavailable (i.e. truly dissolved) chemical fraction [–]										
Freshwater	7.3E-02	8.8E-02	9.9E-01	9.9E-01	2.6E-01	7.3E-02	7.2E-01	9.7E-01	1.0E+00	1.0E+00
HC50: hazard concentration affecting 50% of exposed species [mg/L]										
Freshwater	2.0E-02	1.0E-01	1.5E+00	8.4E-01	1.9E+01	7.7E-01	7.7E-01	1.1E+00	9.3E+00	2.4E+01
ETS: ecotoxicity impact scores [PDF m³ d]										
Freshwater	2.5E+04	1.2E+04	8.9E+03	4.9E+04	2.5E+01	1.5E+03	4.9E+03	3.6E+04	4.5E+03	7.2E+02

[(a)] Cumulative chemical transfer fractions, fractions sent to landfill after product use, and bulk removal rate constants in (continental) freshwater are derived with the PiF modeling framework using the "article interior" module.[5]

[(b)] Bioavailable chemical mass fractions in (continental) freshwater are derived with USEtox.[17]

[(c)] Hazard concentrations are determined based on reported test data as provided in different sources, including USEtox[17] and US EPA's Chemistry Dashboard,[48] or were estimated using a machine learning model.[51] While generally, we recommend deriving effect factors from 0.2/HC20 (see Table 1, main text) in line with current recommendations,[52] we used in our case study 0.5/HC50 as proxy until the HC20-based approach is implemented for the wide range of relevant chemicals.

[(d)] Ecotoxicity impact scores were derived according to Table 1 (main text).

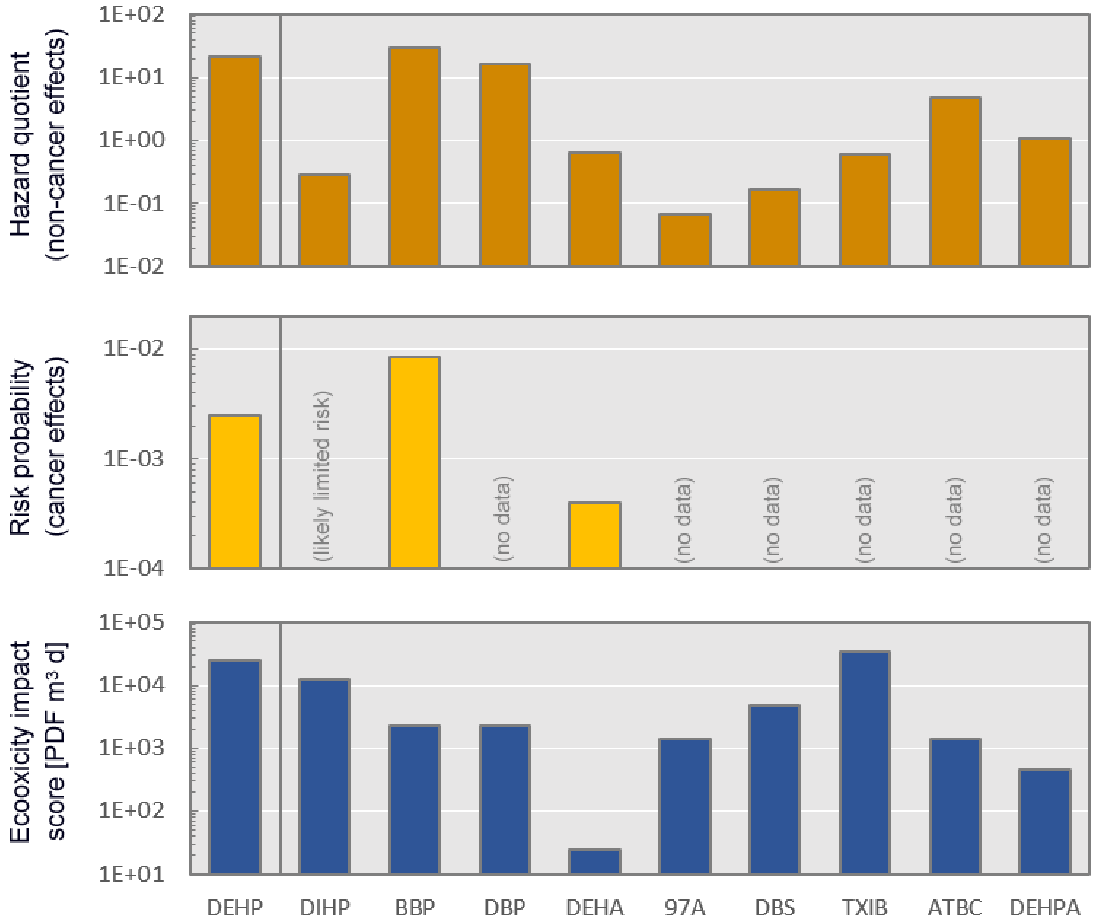

Figure S1. Aggregated product use related non-cancer hazard quotients (top), cancer risk probabilities (middle) and ecotoxicity impacts (bottom) for considered alternative plasticizers in 100 m2 vinyl flooring.

S-8 Chemical supply chain inventory trees for selected plasticizers

For deriving chemical supply chain emissions for three alternative plasticizers in our case study, we used the Environmental Genome of Industrial Processes (EGIP).[14] In EGIP, the publicly available literature is searched for each target chemical to identify the industrial routes, reactants, process equipment, process conditions (temperatures, pressures), and ancillary chemicals like solvents and catalysts. Since ancillary chemicals are often not consumed in significant quantities, these are not generally included in the supply chain, but appear directly in the description of the chemical process. One of the industrially relevant routes is chosen and the reactants for the target chemical become the next target chemicals. The process is repeated until the last target chemicals are elements or materials acquired directly from natural resources (e.g. water, air, or crude oil).

Figure S2 to Figure S4 present a chemical supply chain inventory information tree for producing 1000 kg of a selected plasticizer that was selected in our case study for evaluating chemical supply chain impacts and vinyl flooring life cycle impacts.

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7
2-Ethylhexyl phthalate 1,000	**Ethylhexanol, 2 694**	**Carbon monoxide 312**	**Carbon dioxide 156**	**Natural gas 32.2**	Natural gas (unprocessed) 32.8	
				nitrogen from air 60.0	Air (untreated) 60.0	
				oxygen from air 26.6	Air (untreated) 26.6	
				Water for rxn 41.6	Water (untreated) 41.6	
			Natural gas 105	Natural gas (unprocessed) 107		
			Water for rxn 63.7	Water (untreated) 63.7		
		Hydrogen 39.4	Naphtha 138	oil (in ground) 140		
			Oxygen 138	Air (untreated) 138		
			oxygen from air 90.5	Air (untreated) 90.5		
			Water for rxn 60.0	Water (untreated) 60.0		
		Propylene 469	Naphtha 478	oil (in ground) 485		
	Phthalic anhydride 381	**o-Xylene 320**	Hydrogen 0.514	Naphtha 1.80	oil (in ground) 1.83	
				Oxygen 1.80	Air (untreated) 1.80	
				oxygen from air 1.18	Air (untreated) 1.18	
				Water for rxn 0.784	Water (untreated) 0.784	
			Xylenes 319	**pyrolysis gas 92.6**	Naphtha 94.4	oil (in ground) 95.6
				reformate, from naphtha 227	Naphtha 231	oil (in ground) 234
		oxygen from air 333	Air (untreated) 333			

Figure S2. Chemical supply chain inventory information for producing 1000 kg of DEHP (CAS: 117-81-7) as target chemical (grey box) across seven chemical synthesis integration levels, derived from the Environmental Genome of Industrial Products (EGIP).[14] Orange boxes denote natural resources, normal and bold text/numerical values respectively denote unallocated and allocated processes.

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7
Diisoheptyl phthalate 1,000	**5-Methyl-1-hexanol 652**	4-Methyl-1-Pentene 507	**Propylene 588**	Naphtha 600	oil (in ground) 608	
		Carbon monoxide 135	**Carbon dioxide 67.3**	**Natural gas 13.9**	Natural gas (unprocessed) 14.1	
				nitrogen from air 25.9	Air (untreated) 25.9	
				oxygen from air 11.5	Air (untreated) 11.5	
				Water for rxn 17.9	Water (untreated) 17.9	
			Natural gas 45.4	Natural gas (unprocessed) 46.3		
			Water for rxn 27.5	Water (untreated) 27.5		
		Hydrogen 21.7	Naphtha 76.2	oil (in ground) 77.2		
			Oxygen 76.1	Air (untreated) 76.1		
			oxygen from air 49.9	Air (untreated) 49.9		
			Water for rxn 33.1	Water (untreated) 33.1		
	Phthalic anhydride 410	**o-Xylene 345**	Hydrogen 0.554	Naphtha 1.94	oil (in ground) 1.97	
				Oxygen 1.94	Air (untreated) 1.94	
				oxygen from air 1.27	Air (untreated) 1.27	
				Water for rxn 0.845	Water (untreated) 0.845	
			Xylenes 344	**pyrolysis gas 99.7**	Naphtha 102	oil (in ground) 103
				reformate, from naphtha 245	Naphtha 249	oil (in ground) 252
		oxygen from air 358	Air (untreated) 358			

Figure S3. Chemical supply chain inventory information for producing 1000 kg of DIHP (CAS: 71888-89-6) as target chemical (grey box) across seven chemical synthesis integration levels, derived from the Environmental Genome of Industrial Products (EGIP).[14] Orange boxes denote natural resources, normal and bold text/numerical values respectively denote unallocated and allocated processes.

Level 1	Level 2	Level 3	Level 4	Level 5	Level 6	Level 7	Level 8
bis(2-ethylhexyl)adipate 1,000	**Adipic acid 407**	Cyclohexanol 142	**cyclohexane 129**	**Benzene 120**	**pyrolysis gas 34.8**	Naphtha 35.5	oil (in ground) 36.0
					reformate, from naphtha 85.5	Naphtha 86.8	oil (in ground) 87.9
				Hydrogen 10.6	Naphtha 37.0	oil (in ground) 37.5	
					Oxygen 37.0	Air (untreated) 37.0	
					oxygen from air 24.3	Air (untreated) 24.3	
					Water for rxn 16.1	Water (untreated) 16.1	
			oxygen from air 25.8	Air (untreated) 25.8			
		cyclohexanone 142	**cyclohexane 119**	**Benzene 111**	**pyrolysis gas 32.1**	Naphtha 32.8	oil (in ground) 33.2
					reformate, from naphtha 78.9	Naphtha 80.1	oil (in ground) 81.1
				Hydrogen 9.74	Naphtha 34.2	oil (in ground) 34.6	
					Oxygen 34.1	Air (untreated) 34.1	
					oxygen from air 22.4	Air (untreated) 22.4	
					Water for rxn 14.9	Water (untreated) 14.9	
			oxygen from air 49.3	Air (untreated) 49.3			
		Nitric acid 319	**Ammonia 92.1**	**Natural gas 19.0**	Natural gas (unprocessed) 19.4		
				nitrogen from air 35.4	Air (untreated) 35.4		
				oxygen from air 15.7	Air (untreated) 15.7		
				Water for rxn 24.6	Water (untreated) 24.6		
			Oxygen 517	Air (untreated) 518			
	Ethylhexanol, 2 725	**Carbon monoxide 326**	**Carbon dioxide 163**	**Natural gas 33.6**	Natural gas (unprocessed) 34.3		
				nitrogen from air 62.7	Air (untreated) 62.7		
				oxygen from air 27.8	Air (untreated) 27.8		
				Water for rxn 43.5	Water (untreated) 43.5		
			Natural gas 110	Natural gas 112			
			Water for rxn 66.6	Water (untreated) 66.6			
		Hydrogen 41.2	Naphtha 144	oil (in ground) 146			
			Oxygen 144	Air (untreated) 144			
			oxygen from air 94.6	Air (untreated) 94.6			
			Water for rxn 62.8	Water (untreated) 62.8			
		Propylene 490	Naphtha 500	oil (in ground) 507			

Figure S4. Chemical supply chain inventory information for producing 1000 kg of DEHA (CAS: 103-23-1) as target chemical (grey box) across seven chemical synthesis integration levels, derived from the Environmental Genome of Industrial Products (EGIP).[14] Orange boxes denote natural resources, normal and bold text/numerical values respectively denote unallocated and allocated processes.

S-9 Chemical supply chain impact results

Figure S5 shows case study chemical supply chain impact results for three different plasticizers, which are aggregated into single scores per focus are in Figure S6.

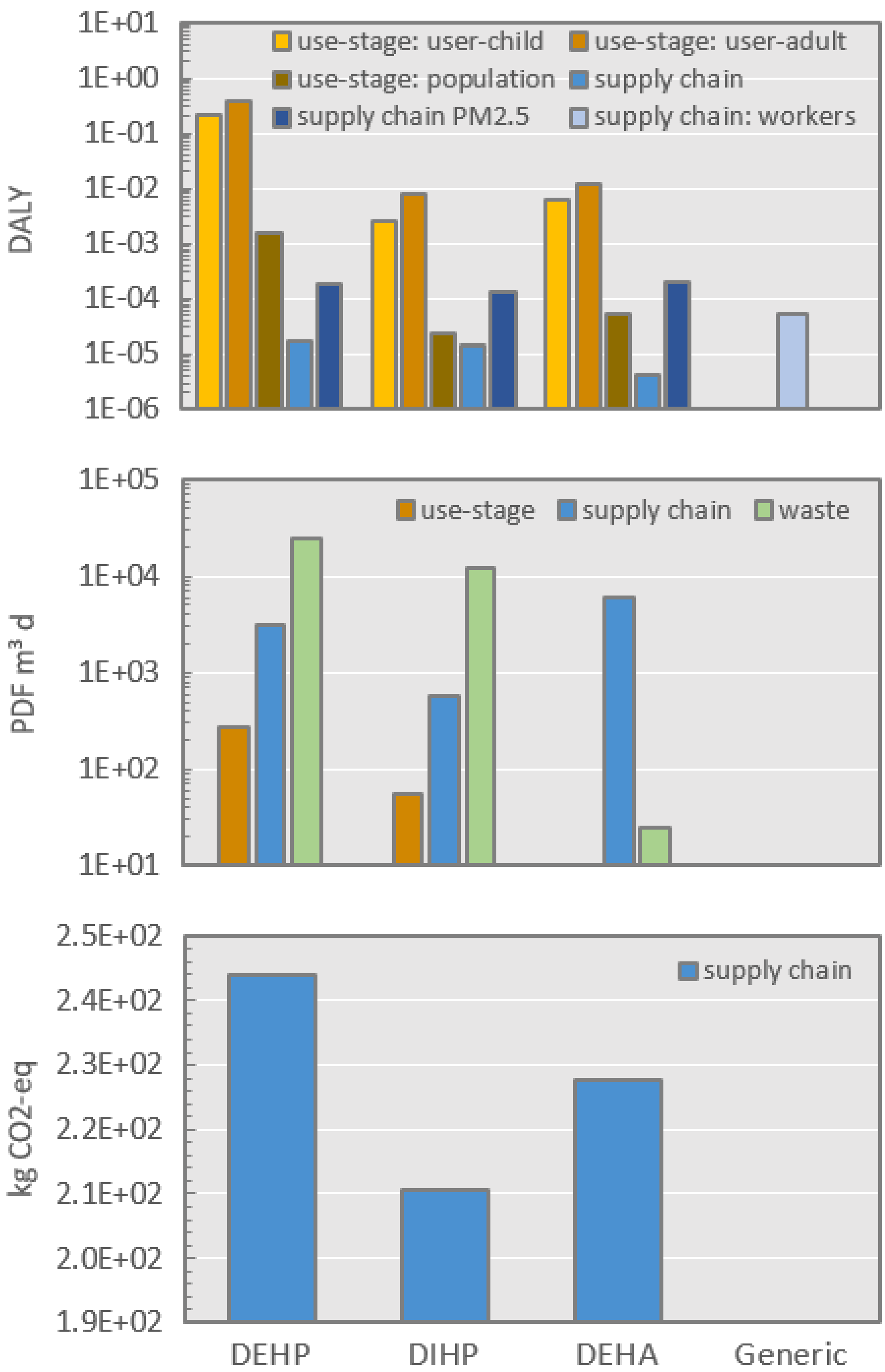

Figure S5. Chemical supply chain impacts expressed as human toxicity and air pollution ($PM_{2.5}$) related damages on human health (top), ecotoxicity damages on ecosystem quality (middle), and climate change impacts (bottom) for three alternative plasticizers in 100 m^2 vinyl flooring.

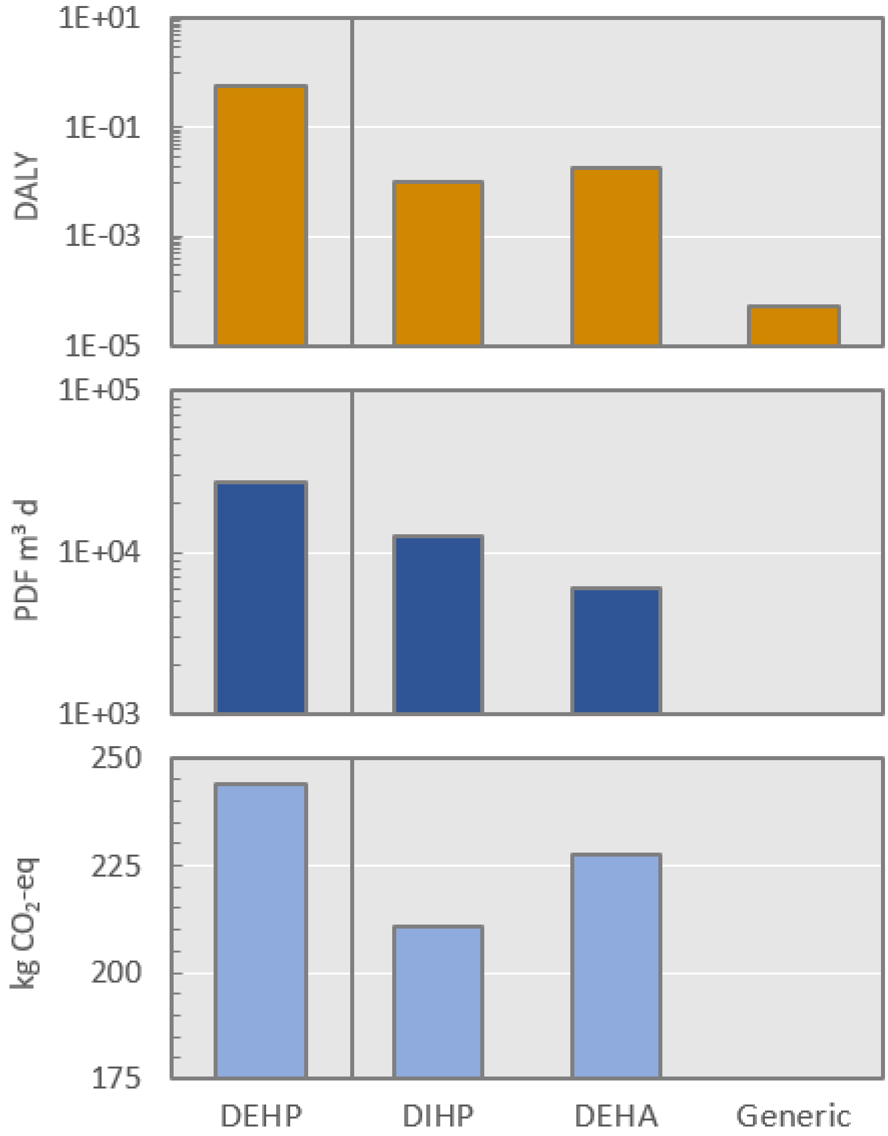

Figure S6. Aggregated chemical supply chain impacts expressed as human toxicity and air pollution ($PM_{2.5}$) related damages on human health (top), ecotoxicity damages on ecosystem quality (middle), and climate change impacts (bottom) for three alternative plasticizers in 100 m^2 vinyl flooring.

S-10 Product life cycle inventory data

Table S9 and Table S10 present vinyl product life cycle inventory data for case study scenarios using three alternative plasticizers in 100 m^2 vinyl flooring. Both tables are provided in a separate Excel file.

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