

Supporting Information

Global Environmental and Toxicological Data of Emerging Plasticizers: Current Knowledge, Regrettable Substitution Dilemma, Green Solution and Future Perspectives

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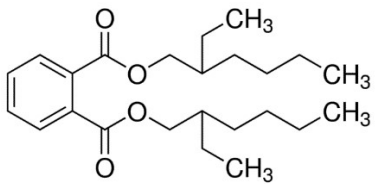
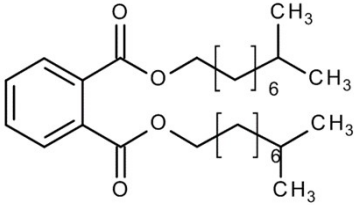
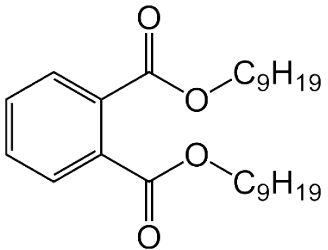
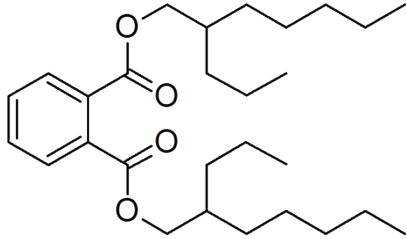
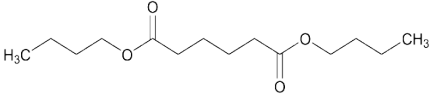
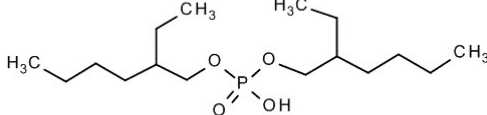
Table S1. Names, abbreviations, and basic properties of phthalates and alternative/emerging plasticizers

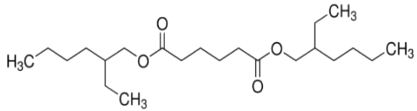
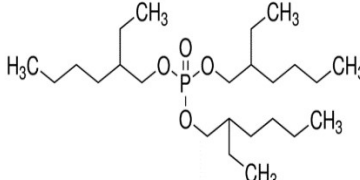
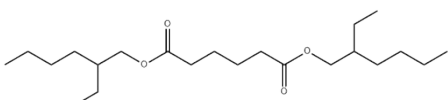
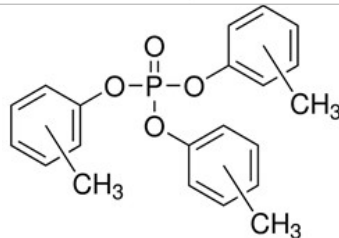
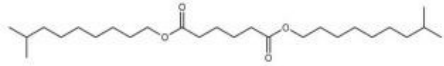
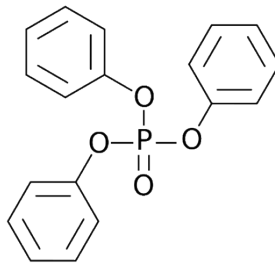
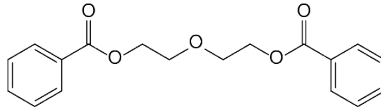
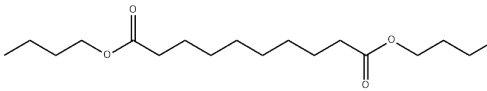
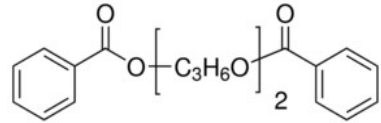
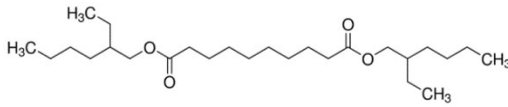
| Name | Abbreviation | Molecular formula | Molecular weight | log Kow (at 25 °C) |
|--|--------------|--|------------------|-----------------------|
| Phthalate plasticizers | | | | |
| Bis-2-ethylhexyl phthalate | DEHP | C ₂₄ H ₃₈ O ₄ | 390.6 | 7.5 |
| Diisononyl phthalate | DINP | C ₂₆ H ₄₂ O ₄ | 418.6 | 9.5 |
| Diisodecyl phthalate | DIDP | C ₂₈ H ₄₆ O ₄ | 446.7 | 9.5 |
| Bis(2-propylheptyl) phthalate | DPHP | C ₂₈ H ₄₆ O ₄ | 446.7 | 10.4 |
| Alternative Plasticizers | | | | |
| (a) Adipates | | | | |
| Dibutyl adipate | DBA | C ₁₄ H ₂₆ O ₄ | 258.3 | 4.3 |
| Bis 2-ethylhexyl adipate | DEHA | C ₂₂ H ₄₂ O ₄ | 370.6 | 8.9 |
| Diisononyl adipate | DINA | C ₂₄ H ₄₆ O ₄ | 398.6 | 9.2 |
| Diisodecyl adipate | DIDA | C ₂₆ H ₅₀ O ₄ | 426.67 | 10.1 |
| (b) Benzoates | | | | |
| Diethylene glycol dibenzoate | DEGDB | C ₁₈ H ₁₈ O ₅ | 314.3 | 3.0 |
| Dipropylene Glycol Dibenzoate | DPGDB | C ₂₀ H ₂₂ O ₅ | 342.4 | 4.3 |
| (c) Citrates | | | | |
| Acetyl tributyl citrate | ATBC | C ₂₀ H ₃₄ O ₈ | 402.5 | 4.3 |
| (d) Cyclohexane dicarboxylic acids | | | | |
| Diisononyl cyclohexane-1,2 dicarboxylate | DINCH | C ₂₆ H ₄₈ O ₄ | 424.7 | 10 |
| (e) Phosphate esters | | | | |

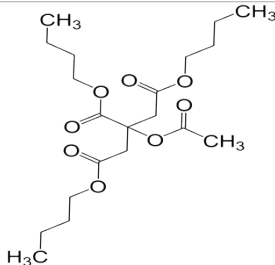
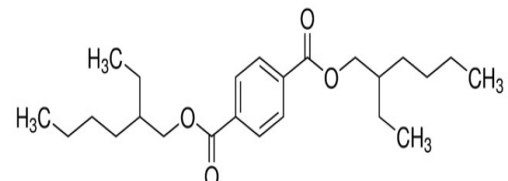
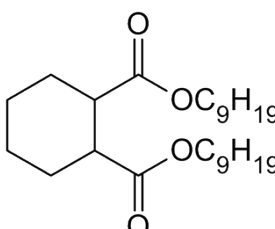
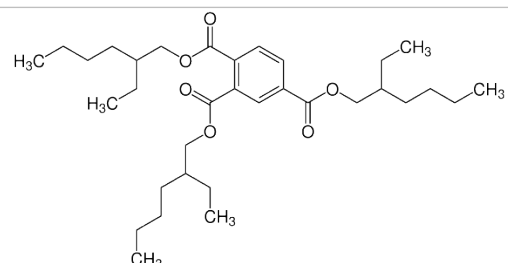
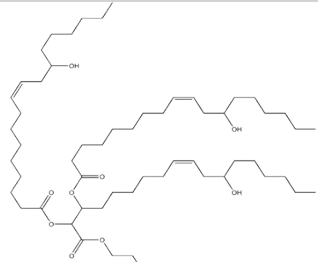
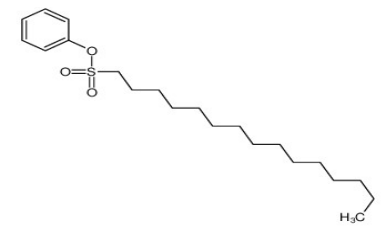
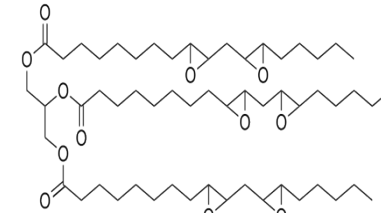
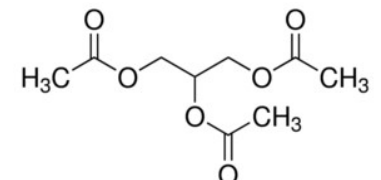
| | | | | |
|--------------------------------------|------------|----------------------|---------|------|
| Bis 2-ethylhexyl phosphate | HDEHP | $C_{16}H_{35}O_4P$ | 322.42 | 2.7 |
| Tris-2-ethylhexyl phosphate | TEHP | $C_{24}H_{51}O_4P$ | 434.63 | 9.5 |
| Tricresyl phosphate | TCP | $C_{21}H_{21}O_4P$ | 368.4 | 5.1 |
| Triphenyl phosphate | TPHP (TPP) | $C_{18}H_{15}O_4P$ | 326.3 | 4.59 |
| (f) Sebacates | | | | |
| Dibutyl sebacate | DBS | $C_{18}H_{34}O_4$ | 314.5 | 6.3 |
| Bis-2-ethylhexyl sebacate | DOS | $C_{26}H_{50}O_4$ | 426.7 | 10.1 |
| (g) Terephthalates | | | | |
| Bis- 2-ethylhexyl terephthalate | DEHT | $C_{24}H_{38}O_4$ | 390.56 | 8.4 |
| (h) Trimellitates | | | | |
| Tris-2-ethylhexyl trimellitate | TOTM | $C_{33}H_{54}O_6$ | 546.78 | 8 |
| f) Vegetable oil derivatives | | | | |
| Castor-oil-mono-hydrogenated acetate | COMGHA | | 500.5 | 6.4 |
| Epoxidized soybean oil | ESBO | $C_{57}H_{98}O_{12}$ | 1000.00 | 14.8 |
| (i) Others | | | | |
| Alkylsulfonic phenyl ester | ASE | N.F | 368.6 | 3.9 |
| Glycerin triacetate | GTA | $C_9H_{14}O_6$ | 218.2 | 0.3 |
| Trimethyl pentanyl diisobutyrate | TXIB | $C_{16}H_{30}O_4$ | 286.4 | 4.9 |

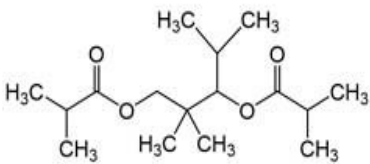
Data was acquired from TOXNET-chemistry database (<https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>)

Table S2. Structures of the phthalate and alternative plasticizers

| Names | Structures | Names | Structures |
|---------------------------------|---|-------------------------|---|
| Phthalate plasticizers | | | |
| DEHP |  | DIDP |  |
| DINP |  | DPHP |  |
| Alternative Plasticizers | | | |
| Adipates | | Phosphate esters | |
| DBA |  | DEHPA |  |

| | | | |
|-----------|---|----------------|---|
| DEHA |  | TEHPA |  |
| DINA |  | TCP |  |
| DIDA |  | TPHP |  |
| Benzoates | | Sebacates | |
| DEGDB |  | DBS |  |
| DPGDB |  | DOS |  |
| Citrates | | Terephthalates | |

| | | | |
|--------------------------------|---|---------------|---|
| ATBC |  | DEHT |  |
| Cyclohexane dicarboxylic acids | | Trimellitates | |
| DINCH |  | TOTM |  |
| Vegetable oil derivatives | | Miscellaneous | |
| COMGHA |  | ASE |  |
| ESBO |  | GTA |  |

| | | | |
|--|--|------|--|
| | | TXIB |  <p>The chemical structure of TXIB is a symmetrical molecule. It features a central carbon atom bonded to two methyl groups (CH₃) and two oxygen atoms. Each oxygen atom is part of an ester linkage to a 2-methylbutanoate group. The 2-methylbutanoate groups are oriented outwards from the central carbon. The central carbon is also bonded to two methyl groups (CH₃) and two oxygen atoms. The 2-methylbutanoate groups are oriented outwards from the central carbon.</p> |
|--|--|------|--|

Structures were taken from chemistry database TOXNET

Table S3. Data of toxicity, exposure, and environment monitoring of plasticizers

| Name | Abbreviations | Toxicological information | Environmental monitoring/exposure | General status of toxicity, exposure and environmental monitoring |
|---------------------------------|---------------|--|---|--|
| Phthalate plasticizers | | | | Generally, data is available [1,2,11–16,3–10] |
| Alternative plasticizers | | | | Generally, lacking data |
| (a) Adipates | | | | |
| Dibutyl adipate | DBA | No data | Concentration (104-839 ug/g) detected in the dust of children's homes [17]. | No data available -No toxicological studies -No ecological studies -One study of environmental monitoring |
| Bis 2-ethylhexyl adipate | DEHA | Endocrine disruption potential in fish [18]. DNA damage in fish [19]. Impairment of the sex steroid homeostasis [20]. Metabolite of DEHA was found to be cytotoxic [21]. Potential carcinogenic and very toxic to aquatic organisms (https://www.cdc.gov/niosh/index.htm). DEHA exposure can lead to fetal death and reduced pregnancies [22]. | Traces found in food and breast milk.[23–25]. Daily DEHA intake was 12.5 µg/day in diet [26]. Traces were found in dust samples of China (max 1520 ng/g) [1]. Kuwait Marine water were found to have 0.06–0.13 µg/L concentration [27]. Swedish preschool dust concentrations were 8.5 µg/g [28]. | Limited data available -Limited toxicological studies -No ecological studies -Limited Environmental monitoring studies |
| Diisononyl adipate | DINA | Potential embryotoxic and disrupts thyroid hormone activity in fish [29]. But according to the Danish Environmental Protection Agency's (DEPA) old report, it is readily biodegradable, no reproductive and developmental toxicity is noticed [30]. | Hospital meals with an estimated daily intake of up to 4.7 µg/day[26]. Concentrations were not detected in retail food.[31] | No data available -One toxicological study (also, Danish Environmental Agency report is available) -No ecological studies |

| | | | | |
|-------------------------------|-------|---|--|--|
| | | | | -One environmental monitoring studies |
| Diisodecyl adipate | DIDA | No Data | Residues (20 ug/l) of DIDA were found in breast milk [25] | No data available -No toxicological studies -No ecological risks studies -No environmental monitoring study (one break milk concentrations available) |
| (b) Benzoates | | | | |
| Diethylene glycol dibenzoate | DEGDB | Possible impairment of lipid metabolism.[32] Potential impact on reproductive health.[30] | No Data | No data available -Limited toxicological studies (old reports) -No Ecological studies -No environmental monitoring studies |
| Dipropylene Glycol Dibenzoate | DPGDB | Low toxicity and no mutagenic effect, according to one old report [33] Potential impact on reproductive health [30] | No Data | No data available -Limited toxicological studies (old reports) -No ecological studies -No environmental monitoring studies |
| (c) Citrates | | | | |
| Acetyl tributyl citrate | ATBC | Abnormal embryo development and disrupted thyroid hormone activity in fish[34]. Potential thyroid hormone disruption in thyroid hormone receptor test [35]. Potential impairment of sex steroid homeostasis [20] Potential detrimental to normal ovarian function in mice.[36,37] | In global water bodies concentrations were 0.05µg/L in the marine environment of Kuwait [27] , <LOQ to 96 ng/L in Nakdong River of Korea [38], 154 µg/L in groundwater of England [39], and ≤ 0.54 in Rur River of Germany[40].Dermal bioaccessibility of ATBC was 75.02 ± 2.12% in house dust [37]. | Limited data available -Few toxicological studies -No ecological studies -Few environmental monitoring studies (few reports indicating their high levels in water bodies around the world) |

| | | | | |
|---|-------|---|--|--|
| | | | Concentrations were found in retail food [31]. High concentrations were found in the home dust of China (max 37,270 ng/g) [1]. | |
| (d) Cyclohexane dicarboxylic acids | | | | |
| Diisononyl cyclohexane-1,2 dicarboxylate | DINCH | <p>Potential physiological and metabolic toxicity in fish [41]. Potential for thyroid hormone disruption in thyroid hormone receptor test [35]. DINCH exposure could impact testosterone levels in humans [42,43]. In vitro study revealed that DINCH can cause cytotoxicity in kidney cells and DNA damage to liver cells [44]. Impairment of metabolic function reduced testosterone levels and damage of the testis in rats [45].</p> <p>Potential endocrine disrupter in silico study [46]. Cytotoxic properties in vitro study.[21] Although considered as non/least toxic by ECHA (2014).</p> | DINCH metabolites (OH-MINCH, cx-MINCH, oxo-MINCH) were found in US population [47], Norway population [48], and German population [49]. Residues of DINCH were found in German house dust upto 110 mg/kg [50]. High levels of residues (ranging 1,060 to 11,550 ng/g) were found in dust samples of China [1]. | <p>Limited data available</p> <ul style="list-style-type: none"> -Few toxicological studies -No ecological studies -Few environmental monitoring studies |
| E) Phosphate esters | | <p>Generally, data is available on toxicity. Conflicting studies on bioaccumulation and biomagnification [51–56]. phosphate esters could cause carcinogenicity, teratogenicity, reproductive issues, and developmental toxicity [53,57–62].</p> | Environmental monitoring worldwide [62–70]. | |
| Bis 2-ethylhexyl phosphate | HDEHP | <p>Potentially can cause irritation and headache. Ecosystem toxicity data indicated it has potential harms to algae, fish, and crustaceans.[71] Potential bioaccumulative substance [71].</p> | <p>Median concentrations were 654 ng/g and 867 ng/g for China and mid-western US dust, respectively [65]. The average concentrations in China were 75 and 31.9 ng/g dw, for Indoor and outdoor dust respectively [72].</p> | <p>Limited data available</p> <ul style="list-style-type: none"> -Limited toxicological studies -No ecological studies -Few environmental monitoring studies |

| | | | | |
|-----------------------------|------|---|--|---|
| Tris-2-ethylhexyl phosphate | TEHP | Potential endocrine disrupter [25,73]. Potential toxicity for <i>Daphnia magna</i> [74]. | Concentrations in Portugal house dust ranged from 250 to 23,000 ng/g [63]. Levels in Swedish preschools dust were 0.44µg/g[28]. | Data available -limited toxicological studies -No ecological studies -Few environmental monitoring studies |
| Tricresyl phosphate | TCP | Exposure of TCP is associated with increased levels of cholesterol and plasma of triglyceride of humans [75]. Potential reproductive toxicant [25]. Potential neurotoxicity, intestinal damage, and DNA damage in earthworms [58]. | High concentrations ranging from 110 to 5200 ng/g were found in house dust [63]. Levels were 0.98 µg/g in Swedish house dust [28]. | Data available -Few toxicological studies -Few ecological studies -Few environmental monitoring studies |
| Triphenyl phosphate | TPHP | Exposure to TPHP is associated with increase cholesterol and plasma levels of triglyceride in humans [75]. Acute toxicity was found to be increased due to the joint effect of TPHP and tributyl phosphate [74]. Potential endocrine disruptor in aquatic organisms and humans [61,76–81]. Only recently, TPHP has been identified as an endocrine disruptor [61,76–81]. | Concentrations were ranged from 110 to 5200 ng/g with 100 percent detection frequency in 28 dust samples of Portugal houses [63]. Average concentrations were 206 and 69.5 ng/g for Indoor and outdoor dust of China, respectively [72]. | Data available -Limited toxicological studies -Few ecological studies -Few environmental monitoring studies |
| (e) Sebacates | | | | |
| Dibutyl sebacate | DBS | No Data | In an old study, concentrations were not detected in Japanese retail food [31].Traces found in polyvinylidene chloride (PVDC) wrapping films [82]. high concentrations of DBS (median 3390 ng/g) in face masks [83]. Likely to found in medicine coating [84]. | No data available -No toxicological studies -No ecological studies - limited environmental monitoring studies |

| | | | | |
|---------------------------------|------|---|--|---|
| Bis-2-ethylhexyl sebacate | DOS | Potentially disrupt thyroid hormone metabolism in fish [85]. | DOS (median 352 ng/g) were found in single-use face masks [83]. | <p>Limited data available</p> <ul style="list-style-type: none"> -One toxicological study -No ecological studies -No environmental monitoring studies |
| (f) Terephthalates | | | | |
| Bis- 2-ethylhexyl terephthalate | DEHT | Bioaccumulation and toxicity in mussels DEHT [86]. Disruptions of post-delivery metabolic health [87]. Potential oxidative stress in an exposed Sertoli cell line [88]. Metabolites were found in adults, nail technicians of USA [89,90], and Portuguese children [91]. Old reports indicated there are no carcinogenic, mutagenic, and developmental defects associated with DEHT.[25,92,93] However, latest investigation is indicating otherwise [93]. Potential endocrine disrupter according to in silico study [46]. | Metabolites of DEHT were quantified in 2970 urine samples of USA adults from 2015 to 2016 [90]. DEHT concentrations were detected in Portuguese children [91]. Concentrations of DEHT (440 mg/kg) were found in dust samples collected from German indoor environments [50]. | <p>Data available</p> <ul style="list-style-type: none"> - Few toxicological studies -Few ecological studies - Few environmental monitoring studies |
| (g) Trimellitates | | | | |
| Tris-2-ethylhexyl trimellitate | TOTM | Human biomonitoring (2014-2017) indicated that children and adolescents had exposure to TOTM.[94] TOTM can cause a low resorption rate and slow metabolism.[95] TOTM exposure can cause estrogen activity and cells[96]. In | High levels of concentrations were found in the dust sample of China, ranging from 404-101,250 ng/g [1]. TOTM was a dominant compound in the sediments of industrialized bays of Korea [100]. | <p>Limited data available</p> <ul style="list-style-type: none"> - Few toxicological studies - No ecological studies - Few environmental monitoring studies |

| | | | | |
|---|--------|---|---|---|
| | | <p>one experiment on mice, exposure to TOTM lead to alternation in cell cycle, oxidative toxicity, and lipid metabolism.[97] Potential endocrine disrupter according to in silico study[46].</p> <p>changes in estrogen activity and cell toxicity in human leukemia and cell assays [96]. Disruption in cell cycle, oxidative stress, and metabolism of lipids in mice [97]. European chemical regulations identify TOTM as the first non-phthalate plasticizer for its potential endocrine disruption, bioaccumulation, and toxic (PBT) properties [98,99].</p> | | |
| Vegetable oil derivatives | | | | |
| Castor-oil-mono-, hydrogenated, acetate | COMGHA | According to ECHA, it is non-hazardous [101]. | No Data | <p>No data available</p> <ul style="list-style-type: none"> - No toxicological studies (one old report) - No ecological studies - No environmental monitoring studies |
| Epoxidized soybean oil | ESBO | British Industrial Biological Research Association (BBIRA) announced ESBO as a low acute toxicant to rats and rabbits [102]. European Chemicals Agency deems ESBO a safe option due to the absence of hazardous properties [101,103,104]. | ESBO ranging from 6 to 100 mg/kg were found in the seven Danish food samples [105]. According to Swiss market survey, ESBO was dominant plasticizer with concentration reached 1,170 mg/g in 158 samples [106]. These values were much higher than migration limit (60mg/kg) set by the European Food Safety Authority [107,108]. | <p>Limited data available</p> <ul style="list-style-type: none"> - Limited toxicological studies (Old reports) - No ecological studies - Few environmental monitoring studies |
| (h) Others | | | | |
| Alkylsulfonic phenyl ester | ASE | Danish Environment Protection Agency reports that ASE exposure was linked to | Elbe river and its tributaries were found to have concentrations from 15 | Limited data available |

| | | | | |
|----------------------------------|------|---|--|---|
| | | low acute toxicity [109] | ug/kg to 33000 ug/kg in sediments.[110] Traces were found in multiple samples of dust and sediments [111,112]. | <ul style="list-style-type: none"> - No toxicological studies (old report) - No ecological studies - Few environmental monitoring studies |
| Glycerin triacetate | GTA | According to US-FDA guidelines, it is generally accepted as safe (GRAS) [113]. No developmental toxicity, carcinogenic effects, and reproductive toxicity effects were found despite lack of quality information [30,113,114]. | No Data | <p style="text-align: center;">Limited data available</p> <ul style="list-style-type: none"> - Limited toxicological studies - No ecological studies - No environmental monitoring studies |
| Trimethyl pentanyl diisobutyrate | TXIB | There are only limited studies (especially peer-reviewed) but also contradictory. In a study involving 203 the repeated application of TXIB did not result in skin sensitization [115]. May cause minor irritation of the eye and nasal mucosa [116]. DEPA states that a 13-week dosing of TXIB in dogs did not lead to harmful effects [30]. When administered orally to rats and rabbits, TXIB demonstrated low acute toxicity, and slight skin irritation in guinea pigs, with no such irritation observed in rabbits [30]. These findings suggest either no toxicity or relatively minimal toxicity. The European Chemical Agency has expressed concerns regarding the potential impact of TXIB on fertility, the developing fetus, and aquatic life with long-lasting effects [117] There are some chances that this compound can be a risk factor of asthma and sick building syndrome [118,119]. Adaptive changes in liver due to exposure of TXIB which | Sweden schools' indoor and outdoor concentrations were 1.64 µg/m ³ and 0.41 µg/m ³ , respectively [121]. | <p style="text-align: center;">Limited data available</p> <ul style="list-style-type: none"> - Limited toxicological studies (old and contradictory reports) - No ecological studies - One environmental monitoring study |

were reversible [120]. Further studies needed.

*Please note due to limited space in the table, it is recommended to read whole article for complete and updated information.

Table S4. Urinary excretion factors (F_{uc}) as DEHTP dose equivalents in %; mean values of three volunteers, ranges in brackets. Data is from[122]

| | 5OH-MEHTP | 5oxo-MEHTP | 5cx-MEPTP | 2cx-MMHTP | Σ all four |
|-------------|------------------|-------------------|--------------------|------------------|--------------------|
| 0–24 h (%) | 1.72 (1.22–2.28) | 0.95 (0.54–1.55) | 12.24 (6.34–19.72) | 0.27 (0.16–0.41) | 15.18 (8.26–23.96) |
| 24–48 h (%) | 0.10 (0.08–0.12) | 0.06 (0.03–0.07) | 0.71 (0.62–0.87) | 0.01 (0.01–0.02) | 0.88 (0.74–1.08) |
| Total (%) | 1.82 (1.34–2.36) | 1.01 (0.57–1.63) | 12.95 (6.96–20.37) | 0.28 (0.17–0.42) | 16.06 (9.04–24.77) |

Table S5 The mean values and ranges of urinary excretion factors, as percentages of the dose on a molar basis, for Hexamoll® DINCH metabolites are provided. Data is from ref [123].

| Time | CHDA | MINCH | OH-MINCH | cx-MINCH | oxo-MINCH | Oxidized metabolites | Over all Σ |
|---------|---------------------|------------------|--------------------|------------------|------------------|----------------------|---------------------|
| 0–24 h | 22.24 (18.83–25.57) | 0.65 (0.26–1.19) | 9.55 (6.64–11.42) | 1.67 (1.38–2.00) | 1.85 (1.39–2.31) | 13.06 (9.41–14.51) | 35.96 (31.99–40.19) |
| 24–48 h | 1.46 (0.97–2.25) | 0.07 (0.06–0.09) | 1.18 (0.88–1.49) | 0.36 (0.29–0.42) | 0.18 (0.14–0.23) | 1.72 (1.16–2.15) | 3.25 (2.20–3.98) |
| 0–48 h | 23.70 (19.98–26.54) | 0.72 (0.31–1.26) | 10.73 (7.70–12.91) | 2.03 (1.75–2.29) | 2.03 (1.52–2.56) | 14.79 (11.29–16.67) | 39.21 (35.86–42.39) |

Table S6. Concentrations (average \pm standard deviation, ng/g ww) of PFRs and plasticizers in black-spotted frog tissues. Data is from [124]

| <i>Tissue</i> | Female Black-Spotted Frogs | | | | | Male Black-Spotted Frogs | | | | |
|---------------|----------------------------|-------------------|-------------------|-------------------|-------------------|--------------------------|-------------------|-------------------|-------------------|-------------------|
| | Liver | Heart | Kidney | Intestine | Lung | Liver | Heart | Kidney | Intestine | Lung |
| <i>N</i> | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| TEP | 0.18 \pm 0.17 | 0.070 \pm 0.030 | 0.16 \pm 0.070 | 0.08 \pm 0.040 | 0.14 \pm 0.060 | 0.040 \pm 0.010 | 0.020 \pm 0.010 | 0.10 \pm 0.010 | 0.030 \pm 0.010 | 0.030 \pm 0.020 |
| TCEP | 2.8 \pm 0.55 | 1.0 \pm 0.44 | 1.4 \pm 0.73 | 0.64 \pm 0.25 | 2.1 \pm 1.1 | 0.89 \pm 0.25 | 0.82 \pm 0.18 | 0.81 \pm 0.32 | 0.58 \pm 0.19 | 0.56 \pm 0.20 |
| TCIPP | 6.0 \pm 0.50 | 0.030 \pm 0.050 | 0.67 \pm 0.38 | 0.30 \pm 0.44 | 1.6 \pm 0.83 | 0.76 \pm 0.78 | 0.72 \pm 0.83 | 1.3 \pm 1.0 | 0.32 \pm 0.070 | 0.29 \pm 0.030 |
| TNBP | 0.68 \pm 0.32 | 0.40 \pm 0.33 | 0.56 \pm 0.73 | 0.16 \pm 0.11 | 0.28 \pm 0.15 | 0.30 \pm 0.12 | 0.070 \pm 0.070 | 0.040 \pm 0.070 | 0.020 \pm 0.020 | 0.040 \pm 0.030 |
| TDCIPP | 1.0 \pm 0.99 | 0.61 \pm 0.38 | 1.0 \pm 0.82 | 0.22 \pm 0.090 | 0.62 \pm 0.59 | 0.010 \pm 0.020 | 0.31 \pm 0.16 | 0.10 \pm 0.11 | 0.040 \pm 0.030 | 0.10 \pm 0.090 |
| TPHP | 0.62 \pm 0.45 | 0.90 \pm 0.75 | 3.4 \pm 3.9 | 0.62 \pm 0.54 | 0.84 \pm 0.43 | 0.14 \pm 0.13 | 0.23 \pm 0.17 | 0.33 \pm 0.060 | 0.27 \pm 0.11 | 0.12 \pm 0.12 |
| TBOEP | 0.29 \pm 0.41 | 0.050 \pm 0.080 | 2.8 \pm 1.7 | 1.2 \pm 2.0 | 0.42 \pm 0.66 | ND | 0.020 \pm 0.030 | 1.5 \pm 1.2 | 0.20 \pm 0.15 | 0.050 \pm 0.050 |
| EHDPPH | 0.99 \pm 1.0 | 0.35 \pm 0.39 | 0.22 \pm 0.12 | 0.13 \pm 0.11 | 0.060 \pm 0.10 | 0.14 \pm 0.13 | 0.090 \pm 0.070 | 0.36 \pm 0.24 | 0.14 \pm 0.060 | 0.12 \pm 0.11 |
| TPTP | 0.050 \pm 0.010 | 0.28 \pm 0.29 | 0.18 \pm 0.10 | 0.060 \pm 0.060 | 0.090 \pm 0.070 | 0.020 \pm 0.020 | 0.060 \pm 0.060 | 0.070 \pm 0.030 | 0.030 \pm 0.010 | 0.020 \pm 0.010 |
| TEHP | 0.15 \pm 0.070 | 0.33 \pm 0.31 | 0.080 \pm 0.070 | 0.070 \pm 0.060 | 0.060 \pm 0.060 | 0.070 \pm 0.080 | 0.080 \pm 0.040 | 0.19 \pm 0.040 | 0.10 \pm 0.010 | 0.060 \pm 0.050 |
| iDDPPH | 0.14 \pm 0.040 | 0.31 \pm 0.25 | 0.46 \pm 0.13 | 0.18 \pm 0.18 | 0.22 \pm 0.11 | 0.050 \pm 0.070 | 0.070 \pm 0.030 | 0.12 \pm 0.050 | 0.040 \pm 0.020 | 0.050 \pm 0.050 |
| RDP | ND | 0.010 \pm 0.010 | 0.020 \pm 0.020 | 0.010 \pm 0.010 | ND | ND | ND | ND | ND | 0.010 \pm 0.010 |
| BDP | 0.15 \pm 0.040 | 0.18 \pm 0.20 | 0.44 \pm 0.36 | 0.12 \pm 0.10 | 0.070 \pm 0.060 | 0.040 \pm 0.060 | 0.010 \pm 0.010 | 0.040 \pm 0.020 | 0.090 \pm 0.15 | 0.010 \pm 0.010 |
| Σ PFRs | 13 \pm 4.6 | 4.50 \pm 3.5 | 11 \pm 9.1 | 3.8 \pm 4.0 | 6.5 \pm 4.2 | 2.5 \pm 1.7 | 2.5 \pm 1.7 | 5.0 \pm 3.1 | 1.9 \pm 0.82 | 1.4 \pm 0.78 |
| DMP | 2.3 \pm 2.5 | 20 \pm 33 | 83 \pm 91 | 25 \pm 19 | 16 \pm 24 | 52 \pm 30 | 33 \pm 18 | 61 \pm 20 | 105 \pm 82 | 55 \pm 29 |
| DEP | 5.7 \pm 3.0 | 57 \pm 82 | 90 \pm 156 | 39 \pm 21 | 6.8 \pm 8.3 | 60 \pm 55 | 31 \pm 11 | 14 \pm 13 | 77 \pm 44 | 52 \pm 45 |

| | | | | | | | | | | |
|----------------------|-------------|-------------|-------------|------------|------------|------------|-----------|-----------|-------------|------------|
| DiBP | 44 ± 33 | 49 ± 29 | 354 ± 472 | 182 ± 77 | 238 ± 213 | 278 ± 180 | 139 ± 51 | 202 ± 59 | 196 ± 47 | 164 ± 73 |
| DnBP | 2066 ± 1816 | 858 ± 1190 | 691 ± 378 | 481 ± 226 | 842 ± 79 | 514 ± 165 | 477 ± 88 | 717 ± 125 | 626 ± 137 | 499 ± 181 |
| BBzP | 1.2 ± 0.77 | 29 ± 49 | 0.62 ± 1.1 | 2.5 ± 4.4 | 1.1 ± 1.5 | 2.2 ± 3.9 | 3.9 ± 3.5 | 1.3 ± 1.6 | 0.15 ± 0.26 | 0.74 ± 1.3 |
| DEHP | 3081 ± 220 | 1443 ± 1311 | 1773 ± 1186 | 884 ± 724 | 1142 ± 400 | 551 ± 362 | 160 ± 11 | 503 ± 229 | 515 ± 366 | 251 ± 100 |
| DEHT | 45 ± 24 | 10 ± 8.0 | 36 ± 49 | 14 ± 6.0 | 26 ± 17 | 4.6 ± 4.2 | 12 ± 12 | 12 ± 9.5 | 24 ± 13 | 26 ± 28 |
| DIDP | 16 ± 2.5 | 28 ± 24 | 64 ± 20 | 84 ± 48 | 88 ± 104 | 4.8 ± 7.0 | ND | ND | 40 ± 17 | 30 ± 22 |
| DINCH | 229 ± 190 | 86 ± 112 | ND | 58 ± 42 | 82 ± 117 | 7.2 ± 7.7 | ND | 45 ± 79 | 81 ± 61 | 40 ± 38 |
| ∑Plasticizers | 5503 ± 2181 | 2584 ± 1601 | 3103 ± 444 | 1772 ± 846 | 2448 ± 822 | 1478 ± 739 | 858 ± 116 | 1561 ± 38 | 1666 ± 701 | 1120 ± 317 |

Table S7. Concentrations (average \pm standard deviation, ng/g ww) of PFRs and plasticizers in bullfrog tissues. Data is from [124]

| Tissues | Female Bullfrogs | | | | | Male Bullfrogs | | | | |
|--|------------------|-------------------|---------------------|-------------------|-------------------|-------------------|-------------------|---------------------|-------------------|-------------------|
| | Liver | Heart | Bullfrogs Kidney | Intestine | Lung | Liver | Heart | Bullfrogs Kidney | Intestine | Lung |
| <i>N</i> | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| TEP | 1.9 \pm 1.8 | 0.070 \pm 0.10 | 0.55 \pm 0.67 | 0.30 \pm 0.23 | 0.060 \pm 0.050 | 0.70 \pm 0.45 | 0.14 \pm 0.20 | 0.53 \pm 0.40 | 0.18 \pm 0.15 | 0.040 \pm 0.050 |
| TCEP | 19 \pm 16 | 4.0 \pm 2.1 | 6.7 \pm 7.2 | 1.6 \pm 1.7 | 1.5 \pm 1.1 | 9.5 \pm 6.6 | 5.3 \pm 2.3 | 4.1 \pm 5.1 | 1.8 \pm 1.7 | 1.1 \pm 1.0 |
| TCIPP | 0.62 \pm 0.22 | 0.77 \pm 0.40 | 0.25 \pm 0.21 | 0.16 \pm 0.15 | 0.16 \pm 0.23 | 0.48 \pm 0.17 | 0.83 \pm 0.25 | 0.25 \pm 0.28 | ND | 0.030 \pm 0.060 |
| TNBP | 0.56 \pm 0.20 | 0.11 \pm 0.050 | 0.10 \pm 0.030 | 0.070 \pm 0.030 | ND | 0.31 \pm 0.21 | 0.090 \pm 0.030 | 0.10 \pm 0.060 | 0.010 \pm 0.030 | ND |
| TDCIPP | 0.59 \pm 0.33 | ND | 0.030 \pm 0.030 | 0.070 \pm 0.040 | 0.050 \pm 0.070 | 0.26 \pm 0.20 | ND | 0.080 \pm 0.070 | 0.050 \pm 0.060 | 0.020 \pm 0.030 |
| TPHP | 17 \pm 25 | 0.010 \pm 0.020 | 1.3 \pm 1.2 | 1.2 \pm 1.1 | 0.56 \pm 0.39 | 1.9 \pm 1.4 | 0.11 \pm 0.12 | 0.79 \pm 0.35 | 0.49 \pm 0.42 | 0.47 \pm 0.30 |
| TBOEP | 2.0 \pm 1.6 | ND | 2.1 \pm 1.7 | 0.75 \pm 0.49 | 0.49 \pm 0.49 | 0.52 \pm 0.46 | 0.030 \pm 0.040 | 1.8 \pm 2.2 | 1.7 \pm 3.0 | 0.89 \pm 1.6 |
| EHDPPH | 0.49 \pm 0.55 | 0.020 \pm 0.030 | 0.86 \pm 0.72 | 0.69 \pm 0.33 | 0.23 \pm 0.31 | 0.29 \pm 0.35 | 0.010 \pm 0.030 | 1.9 \pm 1.9 | 0.27 \pm 0.23 | 0.17 \pm 0.24 |
| TPtP | 1.1 \pm 0.43 | 0.56 \pm 0.22 | 0.57 \pm 0.65 | 0.090 \pm 0.030 | 0.26 \pm 0.21 | 0.84 \pm 0.60 | 0.63 \pm 0.15 | 0.080 \pm 0.10 | 0.11 \pm 0.070 | 0.22 \pm 0.28 |
| TEHP | 0.54 \pm 0.45 | 0.050 \pm 0.040 | 0.16 \pm 0.080 | 0.17 \pm 0.040 | 0.16 \pm 0.11 | 0.23 \pm 0.17 | 0.050 \pm 0.060 | 0.26 \pm 0.21 | 0.18 \pm 0.16 | 0.33 \pm 0.23 |
| iDDPPH | 0.26 \pm 0.45 | ND | 0.040 \pm 0.050 | 0.10 \pm 0.090 | 0.080 \pm 0.12 | 0.080 \pm 0.080 | ND | 0.080 \pm 0.080 | 0.020 \pm 0.030 | 0.040 \pm 0.040 |
| RDP | 0.49 \pm 0.46 | ND | 0.070 \pm 0.060 | 0.13 \pm 0.080 | 0.030 \pm 0.040 | 0.17 \pm 0.16 | ND | 0.18 \pm 0.25 | 0.020 \pm 0.040 | 0.12 \pm 0.24 |
| BDP | 0.76 \pm 0.77 | 0.32 \pm 0.70 | 0.13 \pm 0.070 | 2.3 \pm 4.5 | 0.060 \pm 0.060 | 0.19 \pm 0.19 | ND | 0.37 \pm 0.66 | 0.050 \pm 0.060 | 0.18 \pm 0.23 |
| ΣPFRs | 46 \pm 29 | 5.9 \pm 2.5 | 13 \pm 6.8 | 7.6 \pm 4.1 | 3.6 \pm 1.2 | 16 \pm 4.4 | 7.2 \pm 2.2 | 10 \pm 3.7 | 4.9 \pm 2.8 | 3.6 \pm 1.3 |
| DMP | 23 \pm 12 | 5.5 \pm 4.5 | 45 \pm 34 | 9.7 \pm 4.5 | 14 \pm 12 | 39 \pm 45 | 5.5 \pm 5.5 | 32 \pm 24 | 7.55 \pm 6.2 | 13 \pm 9.6 |
| DEP | 29 \pm 28 | 4.9 \pm 4.7 | 36 \pm 28 | 9.1 \pm 3.8 | 13 \pm 11 | 48.33 \pm 57.39 | 3.1 \pm 3.2 | 29 \pm 26 | 5.36 \pm 3.6 | 12 \pm 7.8 |
| DiBP | 252 \pm 132 | 77 \pm 33 | 731 \pm 624 | 120 \pm 54 | 34 \pm 28 | 435 \pm 748 | 53 \pm 53 | 485 \pm 560 | 97 \pm 73 | 29 \pm 25 |
| DnBP | 1146 \pm 751 | 514 \pm 223 | 609 \pm 161 | 861 \pm 459 | 174 \pm 148 | 766 \pm 821 | 430 \pm 264 | 412 \pm 297 | 412 \pm 339 | 155 \pm 117 |
| BBzP | 8.0 \pm 8.9 | 0.42 \pm 0.57 | 0.51 \pm 0.74 | 1.1 \pm 1.0 | 0.11 \pm 0.14 | 0.85 \pm 0.84 | 0.18 \pm 0.34 | 0.37 \pm 0.59 | 0.13 \pm 0.14 | 0.060 \pm 0.020 |
| DEHP | 1542 \pm 1430 | 74 \pm 96 | 286 \pm 102 | 321 \pm 225 | 96 \pm 101 | 969 \pm 859 | 146 \pm 165 | 707 \pm 352 | 378 \pm 415 | 217 \pm 128 |
| DEHT | 64 \pm 48 | 72 \pm 158 | 18 \pm 8.3 | 25 \pm 20 | 9.6 \pm 8.0 | 30 \pm 32 | 20 \pm 23 | 29 \pm 22 | 20 \pm 16 | 13 \pm 18 |
| DIDP | 128 \pm 109 | 4.3 \pm 5.9 | 56 \pm 45 | 65 \pm 28 | 9.8 \pm 5.9 | 49 \pm 48 | 11 \pm 18 | 53 \pm 40 | 31 \pm 26 | 7.9 \pm 5.8 |
| DINCH | 312 \pm 376 | 0.54 \pm 1.2 | 5.2 \pm 5.6 | 11 \pm 18 | 3.0 \pm 2.4 | 6.3 \pm 7.6 | 3.2 \pm 2.9 | 10 \pm 8.3 | 11 \pm 7.4 | 18 \pm 34 |
| ΣPlasticizers | 3504 \pm 1067 | 753 \pm 487 | 1787 \pm 645 | 1423 \pm 712 | 355 \pm 184 | 2344 \pm 1399 | 672 \pm 487 | 1758 \pm 992 | 961 \pm 819 | 465 \pm 148 |

Table S8. Biological parameters and PFR, PFR metabolites and plasticizer concentrations (ng/g ww, mean \pm standard deviation) for the analyzed organisms. Data is from [125]

| Species | Detection frequency (%) | Water snake | Snake egg | Common carp |
|--|-------------------------|-------------------|--------------------|------------------|
| | | (n= 7) | (n= 3) | (n= 6) |
| Length (cm) | | 44–65 | 0.5–0.8 | 3–5 |
| Weight (g) | | 30–224 | 27–38 | 0.5–1 |
| Lipid (% ww) | | 0.75 \pm 0.22 | 14 \pm 2.3 | 1.2 \pm 0.22 |
| Organophosphorus flame retardants | | | | |
| TEP | 93 | 0.24 \pm 0.21 | 1.0 \pm 0.57 | 0.96 \pm 0.40 |
| TCEP | 93 | 0.046 \pm 0.032 | 0.16 \pm 0.045 | 0.21 \pm 0.10 |
| TCIPP | 100 | 0.31 \pm 0.17 | 0.96 \pm 0.18 | 3.1 \pm 0.48 |
| TNBP | 100 | 0.79 \pm 0.81 | 7.7 \pm 1.4 | 3.0 \pm 1.4 |
| TDCIPP | 47 | 0.32 \pm 0.78 | 0.29 \pm 0.51 | 0.24 \pm 0.21 |
| TPHP | 100 | 0.23 \pm 0.11 | 1.6 \pm 1.7 | 6.2 \pm 1.8 |
| EHDPHP | 47 | ND | 0.61 \pm 0.80 | 0.24 \pm 0.32 |
| TPTP | 53 | ND | 0.011 \pm 0.0070 | 0.21 \pm 0.087 |
| TEHP | 100 | 0.014 \pm 0.011 | 0.11 \pm 0.088 | 0.13 \pm 0.045 |
| Σ_9 PFRs | | 1.9 \pm 1.2 | 12 \pm 2.3 | 14 \pm 2.4 |
| iDDPHP | 47 | 0.049 \pm 0.13 | 0.82 \pm 1.0 | 0.30 \pm 0.36 |
| RDP | 60 | ND | 0.075 \pm 0.088 | 0.45 \pm 0.36 |
| BDP | 93 | 0.16 \pm 0.094 | 0.26 \pm 0.32 | 1.3 \pm 1.1 |
| Σ_3 ePFRs | | 0.22 \pm 0.13 | 1.2 \pm 0.93 | 2.0 \pm 1.2 |
| Plasticizers | | | | |
| DMP | 87 | 0.23 \pm 0.18 | 1.6 \pm 0.55 | 0.25 \pm 0.26 |
| DEP | 53 | 2.2 \pm 3.3 | 20 \pm 14 | 2.7 \pm 4.2 |
| DnBP | 93 | 4.3 \pm 3.2 | 15 \pm 13 | 42 \pm 53 |
| DiBP | 87 | 14 \pm 18 | 35 \pm 13 | 56 \pm 74 |
| DPP | 100 | 0.19 \pm 0.20 | 0.61 \pm 0.36 | 0.24 \pm 0.13 |
| BBzP | 73 | 0.54 \pm 0.59 | 4.2 \pm 1.3 | 0.12 \pm 0.11 |
| DEHP | 100 | 111 \pm 80 | 1191 \pm 327 | 250 \pm 188 |
| Σ_7 LPs | | 132 \pm 76 | 1268 \pm 349 | 351 \pm 169 |
| Alternative Plasticizers | | | | |
| ATEC | 87 | ND | 0.12 \pm 0.047 | 0.32 \pm 0.65 |
| DIBA | 80 | 0.066 \pm 0.11 | 0.61 \pm 0.41 | 1.4 \pm 1.4 |
| CDPHP | 100 | 0.50 \pm 0.23 | 3.1 \pm 1.5 | 4.1 \pm 1.2 |
| ATBC | 20 | 0.37 \pm 0.97 | ND | 13 \pm 19 |

| | | | | |
|------------------------------|-----|---------------|---------------|----------------|
| DBS | 13 | 0.68 ± 1.8 | 5.6 ± 9.8 | ND |
| DEHA | 93 | 3.4 ± 2.9 | 9.2 ± 4.9 | 3.6 ± 1.9 |
| BTHC | 33 | ND | 0.48 ± 0.20 | 0.55 ± 0.77 |
| THTM | 53 | 0.026 ± 0.064 | 1.9 ± 1.2 | 0.42 ± 0.56 |
| TOTM | 93 | 3.6 ± 4.1 | 1.4 ± 1.8 | 9.6 ± 3.1 |
| DEHT | 87 | 3.2 ± 2.7 | 3.4 ± 5.5 | 12 ± 10 |
| DINP | 80 | 3.8 ± 3.0 | 15 ± 26 | 5.8 ± 7.0 |
| DINCH | 73 | 0.27 ± 0.29 | 0.76 ± 1.3 | 2.8 ± 3.2 |
| DIDP | 100 | 1.1 ± 0.77 | 9.6 ± 9.7 | 3.8 ± 2.0 |
| ∑ ₁₃ APs | | 19 ± 7.5 | 52 ± 62 | 59 ± 28 |
| PFR metabolites BCIPP | | | | |
| | 69 | 0.17 ± 0.13 | 0.073 ± 0.13 | 0.54 ± 0.11 |
| DNBP | 92 | 0.47 ± 0.30 | 0.39 ± 0.29 | 0.51 ± 0.32 |
| DPHP | 100 | 0.39 ± 0.37 | 0.50 ± 0.15 | 0.61 ± 0.37 |
| BBOEP | 61 | 0.076 ± 0.12 | 0.29 ± 0.37 | 0.41 ± 0.24 |
| BCIPHIPP | 100 | 0.029 ± 0.013 | 0.037 ± 0.013 | 0.19 ± 0.16 |
| EHPHP | 100 | 0.11 ± 0.033 | 0.32 ± 0.10 | 0.24 ± 0.24 |
| BBOEHEP | 85 | ND | 0.022 ± 0.038 | 0.019 ± 0.010 |
| HO-TBOEP | 100 | ND | 0.031 ± 0.033 | 0.019 ± 0.0090 |
| HO-TPHP | 92 | 0.061 ± 0.057 | 0.28 ± 0.22 | 1.3 ± 1.9 |
| 5-HO-EHDPHP | 31 | ND | 0.046 ± 0.080 | 0.059 ± 0.045 |
| ∑Total metabolites | | 1.3 ± 0.49 | 2.0 ± 0.41 | 2.8 ± 0.41 |

Table S9. Ranges, mean, and standard deviations of OPE concentrations (ng/g dw) detected in fish tissues collected from Laizhou Bay, China. Data is from [126]

| Compound | Muscle | Liver | Kidney | Gill |
|----------|---------------------|---------------------|---------------------|--------------------|
| TMP | nd-2.8 (0.9 ± 0.9) | nd-6.0 (2.6 ± 1.5) | nd-7.4 (2.5 ± 1.7) | nd-3.3 (1.6 ± 0.9) |
| TEP | nd-4.8 (1.9 ± 1.3) | nd-6.1 (3.4 ± 1.5) | nd-10.0 (3.5 ± 2.3) | nd-4.6 (2.6 ± 1.0) |
| TPrP | nd-2.2 (0.6 ± 0.5) | nd-4.2 (1.7 ± 1.2) | nd-3.1 (1.5 ± 0.8) | nd-3.2 (0.8 ± 0.7) |
| TiBP | nd-2.9 (0.8 ± 0.7) | nd-5.2 (1.7 ± 1.3) | nd-2.8 (1.4 ± 0.8) | nd-2.9 (0.9 ± 0.8) |
| TBP | nd-13.1 (4.8 ± 2.9) | nd-12.9 (5.4 ± 3.1) | nd-14.6 (6.2 ± 3.8) | nd-7.6 (4.6 ± 1.7) |
| TCEP | nd-5.8 (1.8 ± 1.7) | nd-8.6 (3.1 ± 2.6) | nd-10.0 (2.9 ± 2.4) | nd-3.3 (1.7 ± 0.9) |
| T CPP | nd-6.1 (1.9 ± 1.8) | nd-9.0 (3.4 ± 3.0) | nd-14.0 (3.6 ± 3.5) | nd-4.0 (2.1 ± 1.2) |
| TPeP | nd-1.9 (0.6 ± 0.6) | nd-6.6 (1.7 ± 1.5) | nd-9.3 (2.2 ± 2.4) | nd-2.7 (0.9 ± 0.6) |
| THP | nd-6.2 (1.2 ± 1.5) | nd-9.0 (2.6 ± 2.5) | nd-7.1 (2.7 ± 1.9) | nd-4.1 (1.2 ± 1.0) |
| TDCIPP | nd-2.5 (0.4 ± 0.5) | nd-6.8 (1.8 ± 1.7) | nd-4.2 (1.6 ± 1.3) | nd-2.2 (0.8 ± 0.6) |
| TBOEP | nd-10.1 (2.3 ± 2.9) | nd-24.7 (4.6 ± 6.0) | nd-17.0 (4.5 ± 4.9) | nd-9.0 (2.9 ± 2.5) |
| TPhP | nd-8.4 (1.6 ± 2.3) | nd-17.3 (4.0 ± 4.2) | nd-14.7 (4.1 ± 4.1) | nd-6.0 (2.7 ± 2.0) |
| EHDP | nd-7.7 (2.7 ± 2.4) | nd-15.2 (4.6 ± 3.7) | nd-11.4 (4.2 ± 3.6) | nd-8.7 (2.9 ± 2.1) |
| TEHP | nd-12.3 (2.6 ± 3.3) | nd-18.4 (4.9 ± 4.6) | nd-16.5 (5.2 ± 5.1) | nd-7.3 (2.1 ± 1.7) |
| CDPP | nd-6.0 (1.2 ± 1.6) | nd-9.3 (2.6 ± 2.0) | nd-6.6 (3.1 ± 2.1) | nd-3.3 (1.4 ± 0.8) |
| TPPO | nd-1.5 (0.5 ± 0.5) | nd-7.2 (1.9 ± 1.6) | nd-4.7 (1.9 ± 1.1) | nd-1.1 (0.7 ± 0.3) |
| TCP | nd-6.0 (1.1 ± 1.4) | nd-9.3 (3.5 ± 2.5) | nd-6.7 (3.1 ± 1.8) | nd-4.2 (1.7 ± 1.1) |

Table S10. Ranges, mean, and standard deviations of OPE concentrations (ng/g lw) detected in fish tissues collected from Laizhou Bay, China. Data is from [126]

| Compound ^a | Muscle | Liver | Kidney | Gill |
|-----------------------|---|--------------------------|---------------------------|--------------------------|
| TMP | nd ^b -147.1 (46.7 ± 39.9) ^c | nd-333.7 (183.4 ± 84.8) | nd-449.5 (192.5 ± 95.6) | nd-212.0 (109.9 ± 58.1) |
| TEP | nd-203.3 (110.3 ± 45.0) | nd-448.0 (246.2 ± 97.6) | nd-603.3 (278.6 ± 130.1) | nd-277.7 (177.4 ± 59.8) |
| TPrP | nd-90.0 (34.2 ± 18.3) | nd-292.4 (118.3 ± 63.8) | nd-205.1 (120.5 ± 51.8) | nd-194.6 (55.1 ± 42.7) |
| TiBP | nd-133.2 (44.3 ± 24.2) | nd-189.7 (111.6 ± 40.2) | nd-198.0 (114.4 ± 51.9) | nd-178.4 (58.9 ± 44.0) |
| TBP | nd-540.1 (295.9 ± 158.8) | nd-706.9 (385.5 ± 159.3) | nd-885.1 (484.7 ± 230.2) | nd-505.4 (317.7 ± 115.1) |
| TCEP | nd-478.7 (114.7 ± 125.4) | nd-734.0 (229.0 ± 199.2) | nd-604.3 (225.8 ± 154.1) | nd-351.7 (133.9 ± 97.3) |
| TCPP | nd-369.2 (116.9 ± 116.2) | nd-739.5 (240.0 ± 206.0) | nd-846.5 (280.6 ± 216.4) | nd-334.7 (159.6 ± 105.3) |
| TPeP | nd-110.1(35.4 ± 34.2) | nd-198.8 (114.5 ± 53.0) | nd-560.5 (175.9 ± 145.2) | nd-150.9 (59.6 ± 34.9) |
| THP | nd-268.5 (62.3 ± 58.1) | nd-497.9 (172.4 ± 116.4) | nd-430.9 (210.7 ± 117.8) | nd-230.3 (77.4 ± 55.5) |
| TDCIPP | nd-221.7 (31.2 ± 51.5) | nd-587.5 (135.1 ± 145.3) | nd-298.7 (119.6 ± 82.9) | nd-230.9 (58.0 ± 54.7) |
| TBOEP | nd-571.4 (145.6 ± 187.2) | nd-742.8 (300.6 ± 232.4) | nd-1026.2 (350.8 ± 309.2) | nd-507.6 (196.8 ± 146.5) |
| TPhP | nd-511.2 (96.6 ± 141.3) | nd-544.6 (266.1 ± 181.2) | nd-888.9 (324.9 ± 287.5) | nd-363.5 (174.6 ± 117.0) |
| EHDP | nd-426.5 (151.1 ± 120.4) | nd-554.0 (298.2 ± 144.1) | nd-689.9 (312.4 ± 205.3) | nd-491.1 (186.2 ± 117.1) |
| TEHP | nd-504.2 (134.6 ± 149.7) | nd-715.0 (324.9 ± 199.6) | nd-999.7 (391.7 ± 303.0) | nd-411.8 (140.0 ± 98.1) |
| CDPP | nd-346.5 (69.4 ± 86.5) | nd-281.4 (180.7 ± 67.1) | nd-474.9 (248.1 ± 142.7) | nd-268.0 (99.7 ± 64.8) |
| TPPO | nd-106.4 (31.2 ± 33.3) | nd-257.6 (124.9 ± 56.8) | nd-284.2 (156.2 ± 68.6) | nd-112.3 (48.7 ± 24.7) |
| TCP | nd-216.3 (59.4 ± 60.0) | nd-487.7 (241.2 ± 97.3) | nd-448.9 (250.5 ± 131.5) | nd-255.3 (114.4 ± 66.1) |

nd= not detected

Table S11. Tissue concentration (ng/g dw) of Σ OPEs, Σ Non-Cl alkyl OPEs, Σ Cl alkyl OPEs, and Σ Aryl-OPEs in 5 benthic fish and 5 pelagic fish species collected from Laizhou Bay. Data is from [126].

| Tissue | Pelagic fish | | | | Benthic Fish | | | | | |
|----------------------------|-------------------|---------------------|------------|------------|-----------------|------------|---------------|-------------|---------------|-------------|
| | Chinese sea perch | Dotted gizzard shad | Halfbeak | Mullet | Silvery pomfret | Eelgoby | Fat greenling | Flathead | Javeline goby | Tongue sole |
| Σ Non-Cl alkyl OPEs | | | | | | | | | | |
| Muscle | 22.4 ± 2.1 | 11.8 ± 1.3 | 3.8 ± 0.5 | 9.6 ± 1.2 | 29.3 ± 6.2 | 9.5 ± 3.1 | 19.6 ± 4.0 | 28.4 ± 3.3 | 13.6 ± 3.2 | 12.9 ± 1.9 |
| Liver | 25.7 ± 3.1 | 19.2 ± 2.6 | 7.9 ± 0.9 | 19.1 ± 2.6 | 39.9 ± 3.5 | 22.6 ± 3.7 | 29.6 ± 5.3 | 59.2 ± 10.2 | 48.8 ± 4.8 | 21.9 ± 3.4 |
| Kidney | 19.4 ± 2.0 | 15.8 ± 1.9 | 10.5 ± 1.6 | 15.9 ± 2.3 | 31.9 ± 3.0 | 17.0 ± 2.6 | 35.2 ± 4.1 | 64.6 ± 9.8 | 22.6 ± 2.7 | 26.7 ± 3.7 |
| Gills | 20.4 ± 2.0 | 10.0 ± 2.0 | 9.1 ± 1.2 | 11.6 ± 2.2 | 25.3 ± 2.2 | 15.0 ± 2.9 | 15.4 ± 2.7 | 36.3 ± 6.3 | 17.4 ± 3.6 | 12.8 ± 3.1 |
| <i>p</i> value | 0.805 | 0.255 | 0.121 | 0.245 | 0.218 | 0.249 | 0.281 | 0.146 | < 0.001 | 0.175 |
| Σ Cl alkyl OPEs | | | | | | | | | | |
| Muscle | 1.1 ± 0.2 | 4.8 ± 4.3 | 0.7 ± 0.3 | 2.4 ± 0.3 | 1.2 ± 0.1 | 13.3 ± 2.6 | 8.2 ± 3.2 | 2.4 ± 0.4 | 2.8 ± 4.3 | 5.7 ± 1.2 |
| Liver | 2.7 ± 0.1 | 8.8 ± 2.8 | 1.7 ± 0.4 | 7.6 ± 2.5 | 3.5 ± 0.6 | 20.7 ± 2.2 | 13.9 ± 6.3 | 7.5 ± 2.7 | 15.9 ± 3.9 | 7.4 ± 1.8 |
| Kidney | 2.7 ± 0.4 | 5.6 ± 1.9 | 2.7 ± 1.1 | 5.9 ± 2.1 | 2.8 ± 0.7 | 14.7 ± 1.8 | 17.0 ± 4.5 | 9.6 ± 2.1 | 8.6 ± 3.6 | 8.9 ± 2.4 |
| Gills | 2.3 ± 0.1 | 4.4 ± 2.6 | 2.0 ± 0.9 | 3.5 ± 1.0 | 4.1 ± 1.1 | 8.7 ± 1.2 | 7.3 ± 3.4 | 5.3 ± 2.5 | 5.5 ± 2.2 | 6.6 ± 2.4 |
| <i>p</i> value | < 0.001 | 0.593 | 0.244 | 0.176 | 0.007 | 0.044 | 0.440 | 0.114 | 0.032 | 0.717 |
| Σ Aryl-OPEs | | | | | | | | | | |
| Muscle | 7.8 ± 1.7 | 1.7 ± 1.2 | 2.1 ± 0.8 | 5.2 ± 0.6 | 13.9 ± 4.4 | 2.6 ± 0.9 | 8.4 ± 2.6 | 15.2 ± 4.0 | 12.8 ± 5.8 | 4.7 ± 1.0 |
| Liver | 15.2 ± 3.2 | 8.5 ± 0.4 | 4.3 ± 0.7 | 12.7 ± 1.5 | 18.3 ± 5.6 | 17.3 ± 2.4 | 15.0 ± 4.0 | 39.1 ± 5.7 | 35.5 ± 4.9 | 10.0 ± 1.3 |
| Kidney | 13.9 ± 2.0 | 5.7 ± 0.1 | 5.1 ± 0.4 | 9.8 ± 1.3 | 15.2 ± 3.9 | 12.3 ± 2.0 | 21.7 ± 2.3 | 32.9 ± 4.8 | 18.2 ± 3.6 | 13.8 ± 2.1 |
| Gills | 12.3 ± 1.1 | 2.5 ± 0.3 | 4.3 ± 0.5 | 6.2 ± 1.6 | 10.5 ± 2.1 | 9.1 ± 1.1 | 7.4 ± 2.1 | 21.9 ± 5.8 | 11.7 ± 2.9 | 4.5 ± 0.8 |
| <i>p</i> value | 0.368 | <0.001 | 0.013 | 0.013 | 0.760 | 0.003 | 0.076 | 0.080 | 0.003 | 0.001 |

Table S12. Mean concentration of OPEs (Cs) measured in seawater, and ranges of Log BAFs in different fish tissues from Laizhou Bay, China. Data is from [126].

| Compound | Cs (ng/L) | log <i>BAF</i> (L/kg wet weight) | | | |
|----------|--------------|----------------------------------|---------------------|---------------------|---------------------|
| | | Muscle | Liver | Kidney | Gill |
| TMP | 6.0 | 1.1-3.2 (2.4 ± 0.6) ^C | 2.7-3.5 (3.2 ± 0.2) | 2.9-3.5 (3.2 ± 0.2) | 2.2-3.2 (2.7 ± 0.3) |
| TEP | 3.9 | 2.8-3.6 (3.2 ± 0.2) | 3.1-3.7 (3.6 ± 0.2) | 3.4-3.8 (3.6 ± 0.2) | 2.9-3.5 (3.2 ± 0.2) |
| TPrP | 1.8 | 2.7-3.5 (3.0 ± 0.3) | 3.0-4.0 (3.5 ± 0.2) | 3.3-3.9 (3.5 ± 0.2) | 2.3-3.2 (3.0 ± 0.3) |
| TIBP | 3.5 | 2.2-3.3 (2.8 ± 0.3) | 2.8-3.7 (3.3 ± 0.2) | 2.8-3.5 (3.2 ± 0.2) | 2.7-3.8 (3.2 ± 0.3) |
| TBP | 15.2 | 2.5-3.3 (3.0 ± 0.2) | 2.7-3.4 (3.1 ± 0.2) | 2.9-3.4 (3.2 ± 0.2) | 2.6-3.8 (3.0 ± 0.3) |
| TCEP | 5.5 | 2.1-3.6 (2.9 ± 0.5) | 2.6-3.8 (3.3 ± 0.4) | 2.8-3.7 (3.3 ± 0.3) | 2.9-4.0 (3.3 ± 0.3) |
| TCPP | 18.8 | 1.8-3.1 (2.4 ± 0.4) | 2.2-3.3 (2.8 ± 0.4) | 2.5-3.2 (2.8 ± 0.3) | 2.0-3.4 (2.7 ± 0.4) |
| TPeP | 1.3 | 1.9-3.7 (3.0 ± 0.7) | 3.3-4.0 (3.7 ± 0.3) | 3.3-3.3 (3.7 ± 0.3) | 3.2-4.3 (3.6 ± 0.4) |
| THP | 1.2 | 2.7-4.1 (3.2 ± 0.4) | 3.3-4.4 (3.8 ± 0.3) | 3.4-4.3 (3.8 ± 0.3) | 2.2-3.4 (2.8 ± 0.4) |
| TDCIPP | 1.6 | 1.5-3.6 (2.7 ± 0.6) | 3.0-4.2 (3.6 ± 0.4) | 3.2-3.0 (3.5 ± 0.3) | 2.5-3.3 (2.9 ± 0.3) |
| TBOEP | 11.7 | 1.3-3.4 (2.6 ± 0.7) | 2.2-3.6 (3.1 ± 0.5) | 2.3-3.7 (3.0 ± 0.4) | 2.0-2.7 (2.5 ± 0.3) |
| TPhP | 6.0 | 1.1-3.7 (2.3 ± 1.1) | 2.6-3.7 (3.3 ± 0.4) | 2.8-3.9 (3.3 ± 0.3) | 2.4-3.6 (3.1 ± 0.4) |
| EHDP | 4.5 | 2.3-3.7 (3.2 ± 0.4) | 2.9-3.8 (3.5 ± 0.3) | 3.0-3.8 (3.5 ± 0.3) | 2.4-3.4 (2.9 ± 0.4) |
| TEHP | 1.0 | 3.0-4.6 (3.8 ± 0.5) | 3.6-4.6 (4.2 ± 0.3) | 3.9-4.7 (4.2 ± 0.3) | 2.7-3.8 (3.1 ± 0.4) |
| CDPP | 0.5 | 2.8-4.4 (3.8 ± 0.6) | 3.9-4.7 (4.4 ± 0.2) | 4.0-4.7 (4.4 ± 0.2) | 3.5-4.3 (3.9 ± 0.3) |
| TPPO | 5.2 | 1.5-3.0 (2.4 ± 0.4) | 2.7-3.5 (3.1 ± 0.2) | 3.0-3.3 (3.2 ± 0.1) | 3.3-4.3 (3.8 ± 0.3) |

| | | | | | |
|-----|-----|---------------------------|---------------------------|---------------------------|---------------------------|
| TCP | 0.6 | 2.8-4.2 (3.6 ± 0.5) | 4.0-4.7 (4.3 ± 0.2) | 4.0-4.5 (4.3 ± 0.2) | 2.3-2.8 (2.5 ± 0.2) |
|-----|-----|---------------------------|---------------------------|---------------------------|---------------------------|

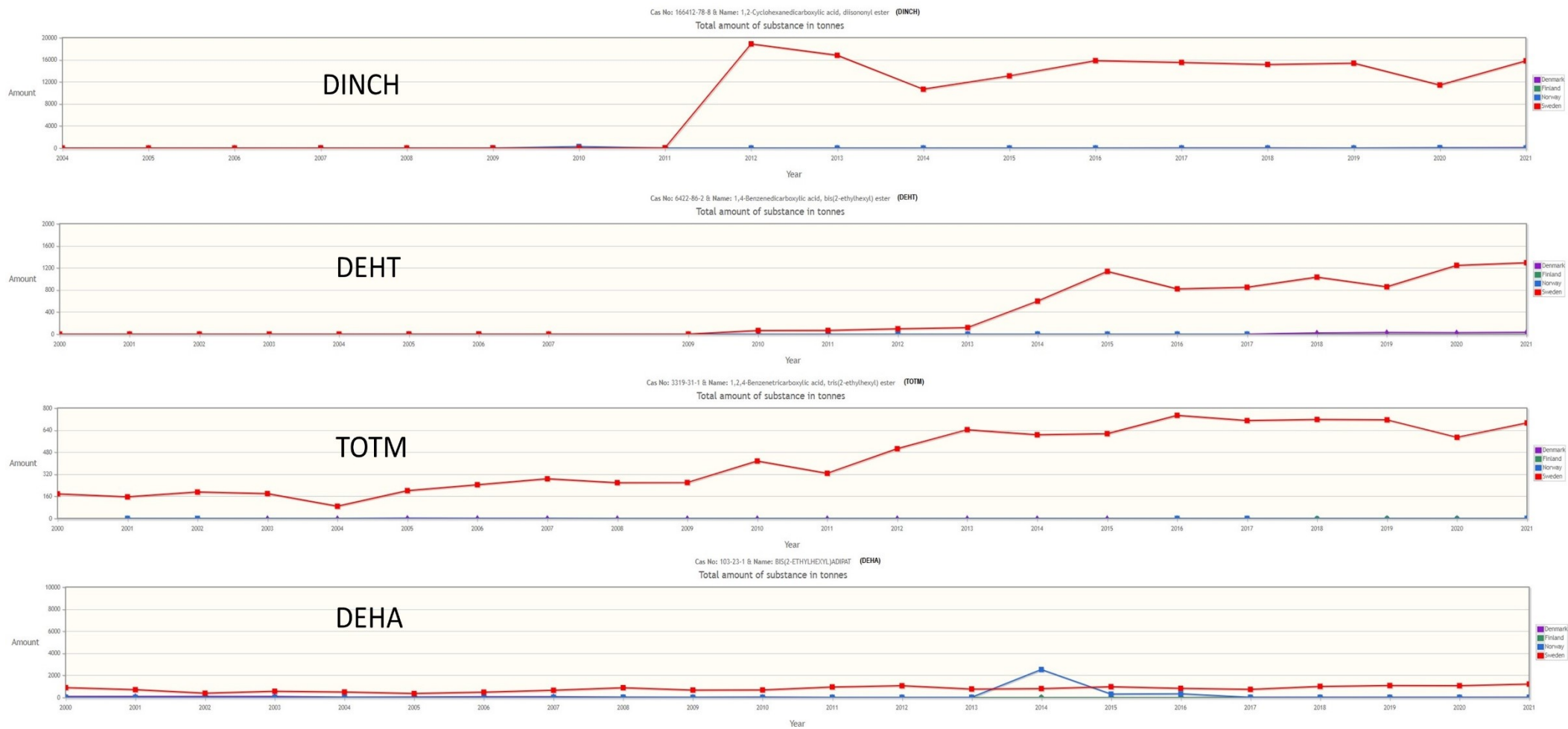


Figure S1. Image indicating that production volumes of few alternative plasticizers is increasing in Nordic Countries. For a clearer view of this image, it is advisable to open it as a whole on separate page. This is from SPIN database (<http://www.spin2000.net/spinmyphp/>)

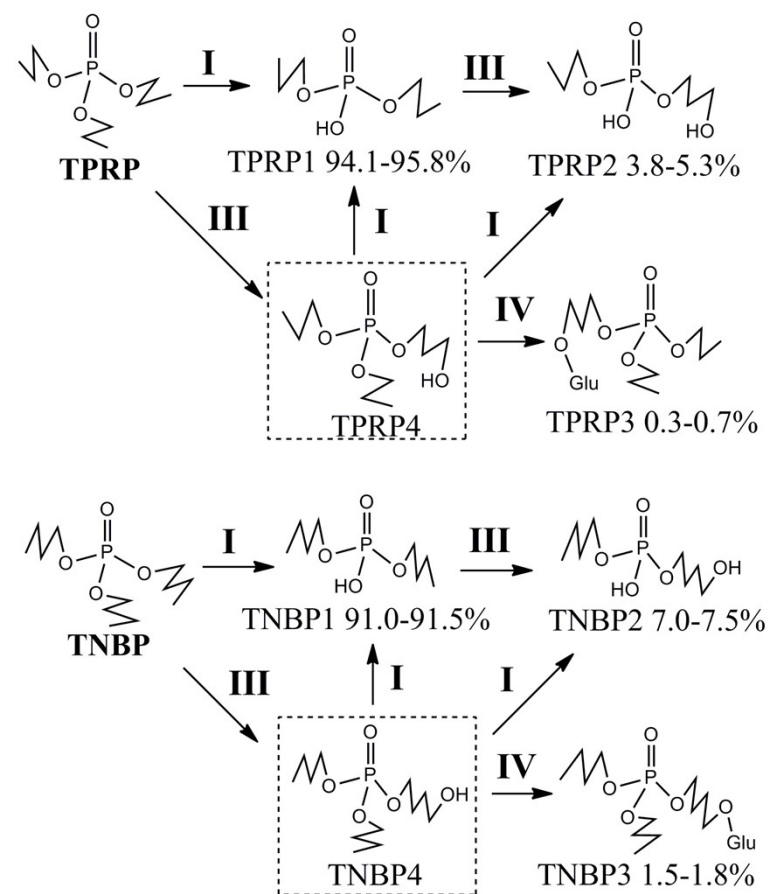


Figure S2. The proposed metabolic pathway of TPRP and TNBP, in zebrafish. I, III, IV, and V are the reaction of scission of the ester bond (or hydrolysis), oxidative hydroxylation, glucuronic acid conjugation, and dechlorination. Contribution of the metabolites was calculated based on the relative peak area of individual metabolite to the total area. Metabolites not detected in liver were framed with dotted boxes. Reprinted with permission from reference ²²² Copyright 2009 Elsevier.

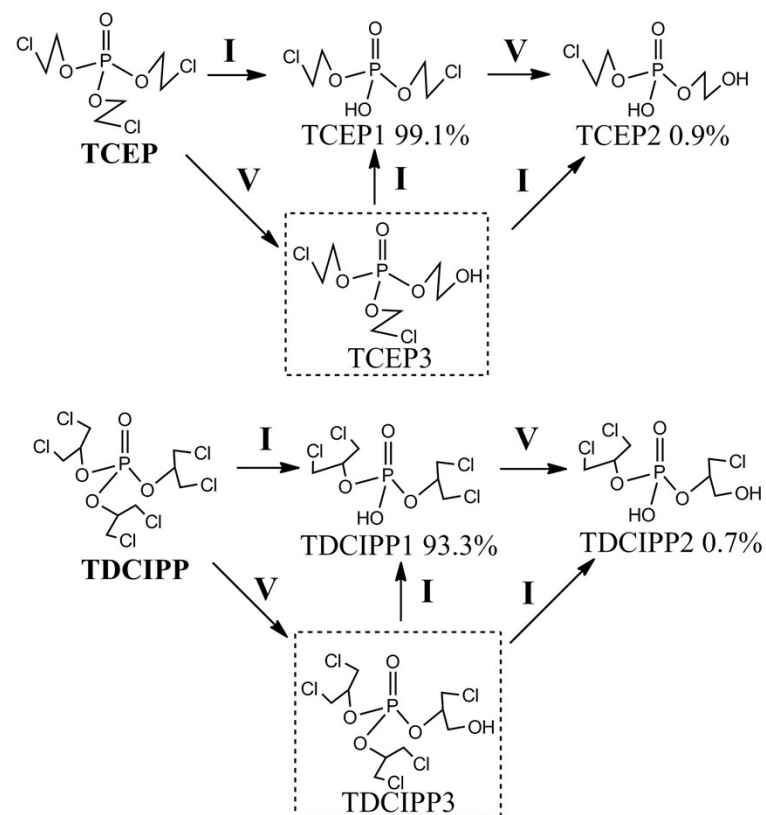


Figure S3. The proposed metabolic pathway of TCEP and TDCIPP, in zebrafish. I, III, IV, and V are the reaction of scission of the ester bond (or hydrolysis), oxidative hydroxylation, glucuronic acid conjugation, and dechlorination. Contribution of the metabolites was calculated based on the relative peak area of individual metabolite to the total area. Metabolites not detected in liver were framed with dotted boxes. Reprinted with permission from reference ²²² Copyright 2009 Elsevier.

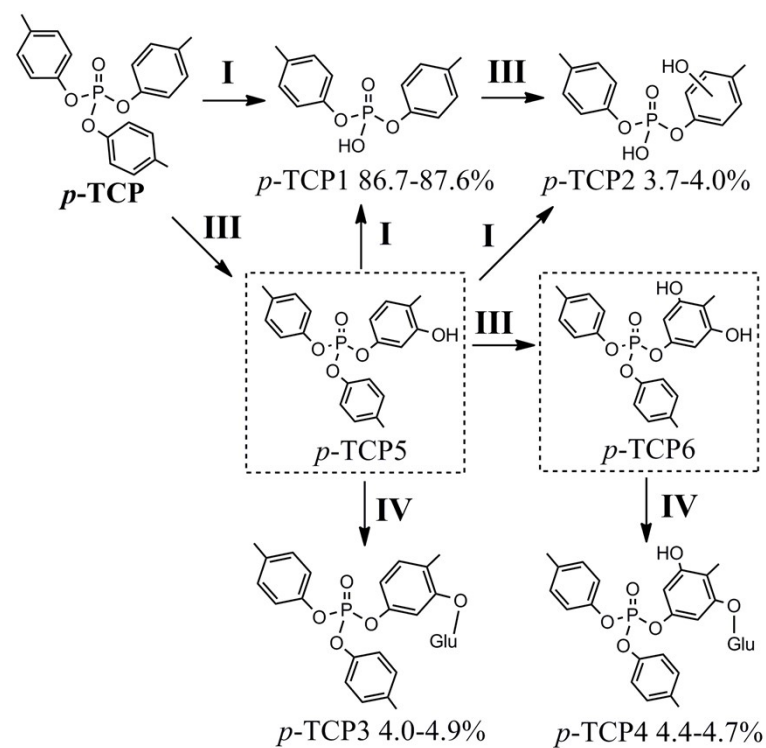


Figure S4. The proposed metabolic pathway of *p*-TCP, in zebrafish. I, III, IV, and V are the reaction of scission of the ester bond (or hydrolysis), oxidative hydroxylation, glucuronic acid conjugation, and dechlorination. Contribution of the metabolites was calculated based on the relative peak area of individual metabolite to the total area. Metabolites not detected in liver were framed with dotted boxes. Reprinted with permission from reference ²²² Copyright 2009 Elsevier.

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