Impact of chemicals regulation: Analysis of industrial use data of plasticizers and patterns of substitution in Scandinavia

* Supplementary material -

*Keywords*: REACH regulation, SPIN database, regrettable substitution, patterns of substitution, chemical hazard burden, sustainable chemistry

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# Identification of water relevant SVHC:

Water relevant substances were defined based on article 16 of the Water Framework Directive (2000/60/EC) as described in the paper. To retrieve industrial use data for water relevant SVHC, the SPIN database was searched for substances from the REACH candidate list (SVHC) with water relevance (substance listed on Water Framework Directive (2000/60/EC) or NORMAN network).10 SVHC have been found on the WFD list. Nine of these substances show end-to-end time trends without any data gaps in SPIN. 20 SVHC have been found on the NORMAN list of emerging substances. Seven of these emerging substances showed end-to-end time trends on SPIN and were therefore considered fit for analysis. In total, 16 SVHC have been identified as water relevant SVHC that had sufficient data considered fit for analysis (Table S1).

Table 1 (S1)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **CAS** | **Name** | **Abbreviation** | **Source** |
| 1 | 104-40-5 | 4-Nonylphenol, branched and linear | 4NP | WFD |
| 2 | 107-06-2 | 1,2-dichloroethane | Dichlorethane | WFD |
| 3 | 117-81-7 | Bis (2-ethylhexyl) phthalate (DEHP) | DEHP | WFD |
| 4 | 140-66-9 | 4-(1,1,3,3-tetramethylbutyl) phenol | Tetramethylbutylphenol | WFD |
| 5 | 25154-52-3 | 4-Nonylphenol, branched and linear, ethoxylated | 4NP, ethoxylated | WFD |
| 6 | 50-32-8 | Benzo[def]chrysene (Benzo[a]pyrene) | Benzo[a]pyrene | WFD |
| 7 | 7440-43-9 | Cadmium | Cadmium | WFD |
| 8 | 79-01-6 | Trichloroethylene | Trichloroethylene | WFD |
| 9 | 85535-84-8 | Short Chain Chlorinated Paraffins | SCCP | WFD |
| 10 | 115-96-8 | Tris(2-chloroethyl) phosphate | TCEP | NORMAN |
| 11 | 85-68-7 | Benzyl butyl phthalate (BBP) | BBP | NORMAN |
| 12 | 84-74-2 | Dibutyl phthalate (DBP) | DBP | NORMAN |
| 13 | 80-05-7 | 4,4'-isopropylidenediphenol Bisphenol A; BPA | BPA | NORMAN |
| 14 | 1163-19-5 | Decabromodiphenyl ether | DecaBDE | NORMAN |
| 15 | 3194-55-6 | Hexabromocyclododecane (HBCDD) | HBCDD | NORMAN |
| 16 | 78-00-2 | Tetraethyllead | Tetraethyllead | NORMAN |

List of 16 water relevant SVHC that originate either from the Water Framework Directive (2000/60/EC) or the list of emerging substances from the NORMAN network.

Water relevant SVHC with an industrial use <10t in 2000 in Sweden were not taken into Figure 2 in the main article to avoid overloading the graph. The raw data for the water relevant SVHC is shown in table 2.

Table 2 (S2)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Time trends showing industrial use of water relevant SVHC in Sweden starting from year 2000 in tons** | | | | | | | | | | | | | | |
| **CAS** | **Name** | **2000 [t]** | **2001 [t]** | **2002 [t]** | **2003 [t]** | **2004 [t]** | **2005 [t]** | **2006 [t]** | **2007 [t]** | **2008 [t]** | **2009[t]** | **2010[t]** | **2011 [t]** | **2012 [t]** | **2013 [t]** | **2014 [t]** |
| 117-81-7 | DEHP | 13226 | 4477 | 2746 | 1658 | 1620 | 1611 | 2102 | 1957 | 1489 | 1105 | 1343 | 449 | 977 | 639 | 1096 |
| 50-32-8 | Benzo[a]pyrene | 1083 | 965 | 985 | 1519 | 1564 | 1064 | 907 | 972 | 901 | 491 | 3143 | 2 | 2 | 2 | 2 |
| 85-68-7 | BBP | 609 | 271 | 693 | 665 | 820 | 727 | 721 | 412 | 20 | 9 | 6 | 9 | 9 | 7 | 7 |
| 79-01-6 | Trichloroethylene | 504 | 381 | 347 | 270 | 214 | 175 | 170 | 152 | 84 | 83 | 81 | 51 | 53 | 31 | 22 |
| 84-74-2 | DBP | 236 | 142 | 174 | 210 | 235 | 210 | 189 | 115 | 69 | 37 | 37 | 35 | 26 | 21 | 8 |
| 80-05-7 | BPA | 91 | 49 | 42 | 43 | 66 | 129 | 130 | 138 | 139 | 55 | 29 | 34 | 18 | 47 | 21 |
| 1163-19-5 | DecaBDE | 89 | 15 | 14 | 5 | 4 | 3 | 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 25154-52-3 | 4NP, ethoxylated | 35 | 12 | 46 | 26 | 10 | 10 | 10 | 14 | 8 | 7 | 8 | 2 | 5 | 27 | 1 |
| 104-40-5 | 4NP | 29 | 16 | 4 | 12 | 7 | 3 | 3 | 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 85535-84-8 | SCCP | 21 | 36 | 18 | 14 | 12 | 12 | 10 | 10 | 10 | 9 | 6 | 4 | 4 | 2 | 1 |
| 115-96-8 | TCEP | 6 | 9 | 17 | 9 | 27 | 38 | 48 | 47 | 1 | 12 | 7 | 1 | 1 | 1 | 1 |
| 140-66-9 | Tetramethylbutylphenol | 6 | 4 | 11 | 7 | 4 | 6 | 7 | 3 | 4 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3194-55-6 | HBCDD | 5 | 59 | 31 | 3 | 4 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 78-00-2 | Tetraethyllead | 5 | 4 | 4 | 3 | 4 | 2 | 2 | 3 | 2 | 6 | 2 | 2 | 2 | 2 | 2 |
| 107-06-2 | Dichloroethane | 1 | 3 | 1 | 1 | 1 | 11 | 4548 | 2576 | 4307 | 3834 | 5912 | 1453 | 2568 | 2578 | 3439 |
| 7440-43-9 | Cadmium | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 70 | 38 | 15 | 1 | 1 | 1 |

Industrial use data from 2000 to 2014 retrieved from the SPIN database for the water relevant SVHC showing their time trends in tpa including substances with a use volume <10t in 2000.

While all other identified water relevant substances were found to decline, 1-2, dichlorethane increased. A possible explaination is that 1-2, dichlorethane is used as an intermediate under strictly controlled conditions reacting to vinyl chloride monomers which is the precursor of polyvinyl chloride (PVC). Under REACH these intermediates are strictly controlled and therefore exempted from authorization, which means that they can be used unrestricted as intermediates. As 80% of the 1-2, dichlorethane is used as intermediated in PVC production, the use data is also not expected to decline. Therefore, 1,2- dichlorethane was exempted from further consideration.

# Selection of PMOCs:

The list of PMOCs was obtained from Schulze et al. as described in the paper. All PMOCs that were used in a volume <10t in Sweden were selected for further analysis (Table S3)

Table 3 (S3)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Time trends showing industrial use of water relevant SVHC in Sweden starting from year 2000 in tons** | | | | | | | | | | | | | | |
| **CAS** | **Name** | **2000**  **[t]** | **2001 [t]** | **2002 [t]** | **2003 [t]** | **2004 [t]** | **2005 [t]** | **2006 [t]** | **2007 [t]** | **2008 [t]** | **2009 [t]** | **2010 [t]** | **2011 [t]** | **2012 [t]** | **2013 [t]** | **2014 [t]** |
| 108-78-1 | Melamin | 8863 | 9290 | 6452 | 8757 | 7196 | 7273 | 4705 | 6883 | 7268 | 7444 | 10621 | 12530 | 6040 | 6641 | 6398 |
| 461-58-5 | Cyanguanidine | 588 | 130 | 1162 | 371 | 409 | 163 | 439 | 479 | 490 | 373 | 416 | 582 | 647 | 548 | 534 |
| 2855-13-2 | Isophoronediamine | 417 | 401 | 423 | 376 | 350 | 339 | 254 | 443 | 437 | 347 | 363 | 438 | 403 | 462 | 481 |
| 140-31-8 | N-Aminoethylpiperazine | 396 | 347 | 474 | 457 | 985 | 1200 | 784 | 166 | 258 | 162 | 188 | 246 | 76 | 83 | 44 |
| 104-15-4 | Toluensulfonic acid | 307 | 368 | 552 | 654 | 551 | 669 | 801 | 928 | 879 | 673 | 778 | 597 | 806 | 302 | 531 |
| 121-57-3 | Sulfanilic acid | 302 | 261 | 0 | 0 | 0 | 0 | 0 | 0 | 771 | 721 | 734 | 935 | 921 | 910 | 686 |
| 13674-84-5 | TCPP | 195 | 145 | 99 | 129 | 81 | 110 | 114 | 121 | 132 | 100 | 84 | 93 | 91 | 129 | 148 |
| 105-60-2 | ε -Caprolactam | 128 | 33 | 95 | 39 | 52 | 23 | 6 | 3 | 3 | 3 | 4 | 5 | 16 | 14 | 42 |
| 3039-83-6 | Sodium Vinylsulfonate | 56 | 73 | 86 | 79 | 92 | 110 | 128 | 143 | 108 | 112 | 158 | 137 | 116 | 110 | 112 |
| 1300-72-7 | Sodium xylenesulfonate | 42 | 35 | 50 | 38 | 72 | 91 | 81 | 64 | 75 | 79 | 82 | 78 | 124 | 77 | 85 |

Industrial use data from 2000 to 2014 retrieved from the SPIN database for PMOCs showing their time trends in tpa including substances with a use volume <10t in 2000.

# Policy framework analysis

Table 4 (S4)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Class** | **Name** | **CAS** | **REACH Annex 14** | **REACH Annex 17** | **Drinking Water Directive** | **PRTR, E-PRTR** | **WFD** | **Other** |
| PMOC | Melamine | 108-78-1 |  |  |  |  |  |  |
| PMOC | Aminoethylpiperazine | 140-31-8 |  |  |  |  |  |  |
| PMOC | Toluene sulfonic acid | 104-15-4 |  |  |  |  |  |  |
| PMOC | Cyanguanidine | 461-58-5 |  |  |  |  |  |  |
| PMOC | Isophoeonediamine | 2855-13-2 |  |  |  |  |  |  |
| PMOC | Benzyldimethylamine | 103-83-3 |  |  |  |  |  |  |
| PMOC | Sodium Vinylsulfonate | 3039-83-6 |  |  |  |  |  |  |
| PMOC | TCPP | 13674-84-5 |  |  |  |  |  |  |
| PMOC | Sodium xylenesulfonate | 1300-72-7 |  |  |  |  |  |  |
| PMOC | ε- Caprolactam | 105-60-2 |  |  |  |  |  | Cosmetic Product Regulation |
| PMOC | Diphenylguanidine | 102-06-7 |  |  |  |  |  |  |
| PMOC | DABCO | 280-57-9 |  |  |  |  |  |  |
| SVHC | DEHP | 117-81-7 | X | x |  | x | x | Cosmetic Product Regulation |
| SVHC | Benzo[a]pyrene | 50-32-8 |  |  |  |  | x | Cosmetic Product Regulation |
| SVHC | BBP | 85-68-7 | X | x |  |  |  | Cosmetic Product Regulation |
| SVHC | DBP | 84-74-2 | X | x |  |  |  | Cosmetic Product Regulation |
| SVHC | Trichloroethylene | 79-01-6 | X |  | x | x | x |  |
| SVHC | Bisphenol A | 80-05-7 |  |  |  |  |  |  |
| SVHC | TCEP | 115-96-8 | X |  |  |  |  | Cosmetic Product Regulation |
| SVHC | SCCPs | 85535-84-8 |  |  |  | x | x | Cosmetic Product Regulation |
| SVHC | 4NP, ethoxylated | 25154-52-3 |  | x |  |  | x | Cosmetic Product Regulation |
| SVHC | 4NP | 104-40-5 |  |  |  |  | x |  |
| SVHC | Tetramethylbutylphenol | 140-66-9 |  |  |  |  | x |  |
| SVHC | DecaBDE | 1163-19-5 |  |  |  |  |  |  |
| SVHC | HBCDD | 3194-55-6 |  |  |  |  | x |  |
| SVHC | Tetraethyllead | 78-00-2 |  |  |  |  |  | Cosmetic Product Regulation, Rotterdam Convention |

Policy framework analysis for unregulated PMOC and under REACH regulated substances of very high concern (SVHC) ensuring regulation status. SVHC are regulated as they are (REACH candidate list) and as seen in the policy framework analysis also regulated under other directives. PMOCs are considered non- regulated as they are rarely regulated under any of the analysed frameworks. In total 21 regulations were considered (S5).

**Legend:**

Reach Annex 14: Authorization list

Reach Annex 17 Restriction list

Drinking Water Directive (98/83/EC)

Ground Water Directive (2006/118/EC)

Protocol on Pollutant Release and Transfer (PRTR, E-PRTR)

Water Framework Directive (2000/60/EC) (WFD priority substances Annex I, WFD priority hazardous substances Annex I)

Table 5 (S5)

|  |
| --- |
| **EU Regulations** |
| Regulation concerning the Registration, Evaluation, Authorization and Restriction of Chemicals (EC/1907/2006) |
| Plant Protection Products Regulation (EC/1107/2009) |
| Biocidal Products Regulation (EC/528/2012) |
| Cosmetic Products Regulation (EC/1223/2009) |
| Regulation on Procedures for the authorization and supervision of Medicinal Products for human and veterinary use and establishing a European Medicines Agency (EC/726/2004) |
| **EU Directives** |
| Water Framework Directive (2000/60/EC) |
| Ground Water Directive (2006/118/EC) |
| Marine Strategy Framework Directive (2008/56/EC) |
| Drinking Water Directive (98/83/EC) |
| Urban Waste Water Treatment Directive (91/271/EEC) |
| Sewage Sludge Directive (86/278/EEC) |
| Industrial Emissions Directive (2010/75/EU) |
| Mining Waste Directive (2006/21/EC) |
| Restriction of the use of certain Hazardous Substances in electric and electronic equipment (2011/65/EU) |
| Toy Safety Directive (2009/48/EC) |
| **Multilateral Environmental Agreements** |
| Stockholm Convention |
| Convention on Long-range Transboundary Air Pollution |
| Protocol on Pollutant Release and Transfer |
| Rotterdam Convention |

21 regulatory frameworks that were considered for the policy framework analysis of PMOCs and SVHC.

# Plasticizer substitutes in Scandinavian countries

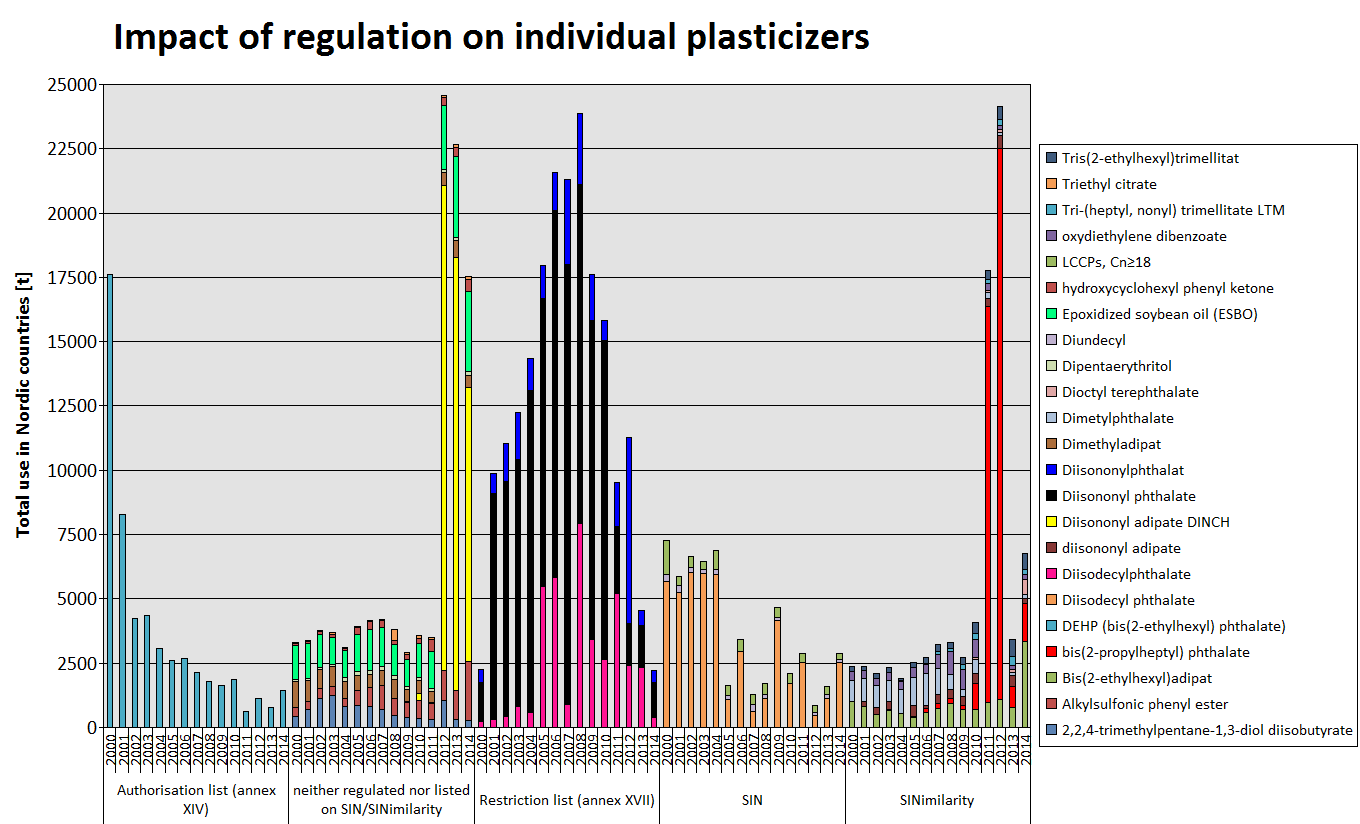


Figure 1 (SF1)

Time trends of industrial use of individual plasticizers in Scandinavia (cumulative data for Norway, Sweden, Finland and Denmark).

# Chemical hazard assessment: Assignment of hazard statements to toxic impact classes

Table 6 (S6)

|  |  |  |
| --- | --- | --- |
| **Hazard class /category under Regulation (EC) No 1272/2008** | **Hazard statement under Regulation (EC) No 1272/2008** | **Human health class** |
| Acute Tox. | H332 | E/D |
| Acute Tox. | H332 | E/D |
| Acute Tox. | H332 | E |
| Acute Tox. | H312 | E/D |
| Acute Tox. | H302 | E/D |
| Acute Tox. | H331 | D/C |
| Acute Tox. | H330 | D |
| Acute Tox. | H331 | D/C |
| Acute Tox. | H311 | D/C |
| Acute Tox. | H301 | D/C |
| Acute Tox. | H330 | C |
| Acute Tox. | H330 | C |
| Acute Tox. | H330 | C |
| Acute Tox. | H310 | C |
| Acute Tox. | H300 | C |
| STOT RE 2 | H373 | D |
| Skin Corr. | H314 | D |
| Skin Corr. | H314 | C |
| Eye Irrit. 2 | H319 | E |
| STOT SE 3 | H335 | E |
| Skin Irrit. 2 | H315 | E |
| STOT SE 1 | H370 | D |
| STOT SE 1 | H370 | D |
| STOT SE 1 | H370 | D |
| STOT SE 1 | H370 | C |
| STOT SE 1 | H370 | C |
| STOT SE 1 | H370 | C |
| Eye Dam. 1 | H318 | D |
| Resp. Sens. 1 | H334 | B |
| Skin Sens. 1 | H317 | B |
| STOT RE 2 | H373 | D |
| STOT RE 2 | H373 | D |
| STOT RE 2 | H373 | D |
| STOT RE 1 | H372 | C |
| STOT RE 1 | H372 | C |
| STOT RE 1 | H372 | C |
| Lact. | H362 | B |
| Asp. Tox. 1 | H304 | E |
| STOT SE 3 | H336 | E |
| STOT SE 2 | H371 | E |
| STOT SE 2 | H371 | E |
| STOT SE 2 | H371 | E |
| Carc. 1A | H350 | A |
| Carc. 1B | H350 | A |
| Carc. 1A | H350 | A |
| Carc. 1B | H350 | A |
| Carc. 2 | H351 | B |
| Muta. 1A | H340 | A |
| Muta. 1B | H340 | A |
| Muta. 2 | H341 | B |
| Repr. 1A | H360 | A |
| Repr. 1B | H360 | A |
| Repr. 1A | H360 | A |
| Repr. 1B | H360 | A |
| Repr. 2 | H361f | B |
| Repr. 2 | H361d | B |
| Repr. 1A | H360FD | A |
| Repr. 1A | H360FD | A |
| Repr. 1A | H360FD | A |
| Repr. 1B | H360FD | A |
| Repr. 2 | H361fd | B |
| Repr. 1A | H360Fd | A |
| Repr. 1B | H360Fd | A |
| Repr. 1A | H360Df | A |
| Repr. 1B | H360Df | A |

Assignment of H- statements to human health hazard classes according to an existing methodology by Oltmans et. al as described in paper. According to the methodology, any of these human health hazard statements leas to class E in environmental hazard, even if the substance is not classified for environmental hazards.

Table 7 (S7)

|  |  |  |
| --- | --- | --- |
| **Hazard class /category under Regulation (EC) No 1272/2008** | **H- statement** | **Environmental hazard class** |
| Aquatic Acute 1 | H400; H410 | A |
| Aquatic Chronic 2 | H411 | B |
| Aquatic Chronic 3 | H412 | C |
| Aquatic Chronic 4 | H413 | D |
| Aquatic Chronic 4 | H413 and log Kow 5.2-6.0 | A |

Assignment of H- statements to environmental hazard classes according to methodology derived from Eurostat (Eurostat, 2016).

Table 8 (S8)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Hazard Class** | **A** | **B** | **C** | **D** | **E** |
| **Human health** | CMR chemicals | Chronic toxic chemicals | Very toxic chemicals | Toxic chemicals | Harmful chemicals |
| **Environment** | Severe chronic environmental hazard | Significant chronic environmental hazard | Moderate chronic environmental hazard | Chronic environmental hazard | Significant acute environmental hazard |

Labelling of hazard classes.