Supporting Information

for

Screening organic chemicals in commerce for emissions in the context of environmental and human exposure

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Methods (continued)

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Estimating total quantities in commerce from the HPV lists

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31 We initially calculated the sum of B_{MAX} and B_{MIN} for chemicals which appeared on the US, Japanese
32 and/or highly resolved European lists only ($\Sigma_3 B_{MIN}$, $\Sigma_3 B_{MAX}$), furthermore excluding substances which
33 were included into the top bin on any of these lists (those without upper brackets defined). The
34 resulting ranges across these lists ($\Sigma_3 B_{MAX} - \Sigma_3 B_{MIN}$) for any chemical considered were always 2.02 log
35 units or less (N=10,236). As a first approximation, we assumed that any missing brackets would be
36 anticipated to be no more than about 2 orders of magnitude higher (or lower) than B_{MIN} (or B_{MAX}) for the
37 corresponding bin. This "empirical" range was in turn derived to estimate B_{MAX} for the upper bins as well
38 as B_{MIN} on the US list. As the pre-defined range for the lower bin on the Canadian list (1-10^3 t/yr)
39 exceeded the empirical range derived above, the same range (2.02 log units) was also applied in this
40 specific case to derive a revised estimate for B_{MAX} for this bin whenever (i) a given chemical was included
41 into this bin on the Canadian list only (which would indicate that the chemical was more likely to belong
42 into the lower end of this bin), or (ii) the sum of B_{MAX} for the European, US and Japanese lists constituted
43 less than 10 t/yr (i.e. < 1% of the pre-defined B_{MAX} value of 1000 t/yr on the Canadian list). This
44 correction was made to reduce the risk of significantly overestimating B_{MAX} for chemicals belonging to
45 the Canadian bin under circumstances when quantities were relatively minor on the other lists. The sum
46 of the resulting upper and lower brackets from the US, European, Japanese and Canadian lists ($\Sigma_4 B_{MIN}$,
47 $\Sigma_4 B_{MAX}$) were then derived for all substances and compared with the OECD data. If the substance also
48 appeared on the OECD list (>10^3 t/yr) and, (i) $\Sigma_4 B_{MIN}$ was less than 10^3 t/yr, then 10^3 t/yr were used as
49 the minimum quantity (Q_{MIN}), (ii) if the estimated upper bracket on the OECD list (i.e. $10^{5.02}$) exceeded
50 $\Sigma_4 B_{MAX}$, then the maximum quantity (Q_{MAX}) was assumed equal to $10^{5.02}$. Otherwise, Q_{MIN} and Q_{MAX} were
51 assumed equal to $\Sigma_4 B_{MIN}$ and $\Sigma_4 B_{MAX}$, respectively.

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60   Table S1. Industrial Categories discriminated in the EU TGD (ECB, 2003).

IC	Definition
1	Agricultural industry
2	Chemical industry: Basic chemicals
s3	Chemical industry: Chemicals used in synthesis
4	Electrical/electronic industry
5	Personal/domestic
6	Public domain
7	Leather processing industry
8	Metal extraction, refining and processing industry
9	Mineral oil and fuel industry
10	Photographic industry
11	Polymers industry
12	Pulp, paper and board industry
13	Textile processing industry
14	Paints, lacquers and varnishes industry
15 (0)	Others
16	Engineering industry: civil and mechanical

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62   Table S2. Use Categories discriminated in the EU TGD (ECB, 2003).

UC	Definition
1	Absorbents and adsorbents
2	Adhesive, binding agents
3	Aerosol propellants
4	Anti-condensation agents
5	Anti-freezing agents
6	Anti-set-off and anti-adhesive agents
7	Anti-static agents
8	Bleaching agents
9	Cleaning/washing agents and additives
10	Colouring agents
11	Complexing agents
12	Conductive agents
13	Construction materials and additives
14	Corrosion inhibitors
15	Cosmetics
16	Dust binding agents
17	Electroplating agents
18	Explosives
19	Fertilisers

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65   Table S2 (cont. from previous page)

UC	Definition
20	Fillers
21	Fixing agents
22	Flame retardants and fire preventing agents
23	Flotation agents
24	Flux agents for casting
25	Foaming agents
26	Food/feedstuff additives
27	Fuels
28	Fuel additives
29	Heat transferring agents
30	Hydraulic fluids and additives
31	Impregnation agents
32	Insulating materials
33	Intermediates
34	Laboratory chemicals
35	Lubricants and additives
36	Odour agents
37	Oxidising agents
38	Plant protection products, agricultural
39	Biocides, non-agricultural
40	pH-regulating agents
41	Pharmaceuticals
42	Photochemicals
43	Process regulators
44	Reducing agents
45	Reprographic agents
46	Semiconductors
47	Softeners
48	Solvents
49	Stabilisers
50	Surface-active agents
51	Tanning agents
52	Viscosity adjustors
53	Vulcanising agents
54	Welding and soldering agents
55 (0)	Other

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70 Table S3. Frequency distribution for valid IC/UC categories among European HPV substances (in
71 %).

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0	0.17	0.19	0	0	0	0	0	0	0	0	0	0	0	0.18	0
2	0	0	0	0.19	0.50	0.36	0	0	0	0	0	0.50	0	0	0.82	0
3	0.04	0	0	0	0.27	0	0	0	0	0	0	0	0	0.07	0.25	0
4	0	0.02	0.02	0	0	0	0	0	0	0	0	0	0	0.02	0.02	0
5	0	0.21	0.22	0	0.13	0	0	0	0.09	0	0	0	0	0	0.19	0
6	0	0.06	0.04	0	0.05	0.01	0.04	0	0	0	0.07	0.07	0.04	0	0.06	0
7	0	0.09	0.13	0.01	0.15	0	0	0	0.04	0	0.15	0	0.12	0	0.16	0
8	0	0.06	0.09	0	0.11	0	0.05	0	0	0.04	0	0	0.09	0	0.07	0
9	0.42	0	0	0.25	1.39	0.92	0.36	0.29	0	0	0.62	0.41	0.79	0	0.99	0
10	0.15	0	0	0.06	0.15	0	0.07	0	0.10	0.06	0.30	0.16	0.34	0.40	0.29	0
11	0	0	0	0	0.16	0	0	0	0	0	0	0	0	0	0.25	0
12	0	0.02	0.01	0.01	0	0	0	0	0	0	0	0	0	0	0.05	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.40	0
14	0	0	0	0	0.25	0	0	0.13	0	0	0	0	0	0.28	0.36	0
15	0	0	0	0	1.42	0	0	0	0	0	0	0	0	0	0.98	0
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.11	0
17	0	0	0	0.02	0	0	0	0.02	0	0	0	0	0	0	0.04	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.13	0
19	0.16	0	0	0	0.11	0.06	0	0	0	0	0	0	0	0	0.16	0
20	0	0	0	0	0	0	0	0	0	0	0.11	0.11	0	0.16	0.15	0
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.09	0
22	0	0	0	0.02	0	0	0	0	0	0	0.22	0	0.11	0	0.19	0
23	0	0	0	0	0	0	0	0.12	0	0	0	0.02	0	0	0.12	0
24	0	0	0	0	0	0	0	0.02	0	0	0.01	0	0	0	0.02	0
25	0	0	0	0	0	0	0	0	0	0	0.19	0	0	0	0.16	0
26	0.27	0	0	0	0.59	0	0	0	0	0	0	0	0	0	0.57	0
27	0	0	0	0	0.46	0.25	0	0	1.31	0	0	0	0	0	1.08	0
28	0	0	0	0	0.10	0.07	0	0	0.33	0	0	0	0	0	0.29	0
29	0	0	0	0.10	0	0	0	0.07	0	0	0	0	0	0	0.30	0
30	0.18	0	0	0	0	0	0	0	0	0	0	0	0	0	0.39	0
31	0	0	0	0.06	0	0	0.10	0	0	0	0	0.16	0.15	0	0.31	0
32	0	0	0	0.06	0.13	0.07	0	0	0	0	0	0	0	0	0.18	0
33	0	0	5.00	0	0	0	0	0	2.08	0	2.39	0	0	0	3.36	0
34	0	0.52	0.53	0	0	0	0	0	0	0	0	0	0	0	0.48	0
35	0.30	0	0	0	0.53	0.33	0	0.33	0	0	0.94	0	0	0	1.15	0
36	0.11	0	0	0	0.63	0	0	0	0	0	0	0	0	0	0.24	0
37	0	0.06	0.09	0	0	0	0	0	0	0	0	0	0	0.04	0.07	0
38	0.74	0	0	0	0.31	0.27	0	0	0	0	0	0	0	0	0.64	0
39	0.13	0	0	0	0.15	0.11	0.06	0.05	0	0	0	0.07	0	0	0.16	0
40	0	0.22	0.25	0	0	0	0	0	0	0	0	0	0	0	0.23	0
41	0.36	0	0	0	0.68	0	0	0	0	0	0	0	0	0.59	0.98	0

42	0	0	0	0.09	0	0	0	0	0	0.25	0	0	0	0	0.21	0
43	0	0.31	0.53	0	0	0	0	0	0	0	0.44	0	0	0	0.33	0
44	0	0.05	0.10	0	0	0	0	0	0	0	0	0	0	0	0.05	0
45	0	0	0	0	0	0	0	0	0	0	0	0.05	0	0	0.12	0
46	0	0	0	0.02	0	0	0	0	0	0	0	0	0	0	0.02	0
47	0	0	0	0	0.36	0	0	0	0	0	0.64	0	0	0.45	0.53	0
48	0.46	1.63	1.60	0.30	0.94	0.61	0	0.27	0	0	0.97	0.28	0.61	1.44	1.21	0
49	0	0.29	0.44	0	0	0	0	0	0.09	0	0.42	0	0	0	0.35	0
50	0.18	0.31	0.51	0.09	0.51	0.28	0	0.16	0	0	0	0	0.41	0.30	0.42	0
51	0	0.13	0.17	0	0	0	0.19	0	0	0	0	0	0	0	0.15	0
52	0	0	0	0	0	0	0	0	0.13	0	0	0	0	0.22	0.22	0
53	0	0	0	0	0	0	0	0	0	0	0.30	0	0	0	0.30	0
54	0	0	0	0.02	0	0	0	0.05	0	0	0	0	0	0	0.05	0
55	0.90	2.62	3.74	0.36	1.96	1.06	0.46	0.63	1.87	0	2.60	0.83	1.33	2.06	3.57	0

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References (SI)

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76 ECB. Technical Guidance Document on Risk Assessment: European Chemicals Bureau; 2003

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