

**Supplementary Material for**

**Evaluating consumer exposure to disinfecting chemicals against coronavirus disease 2019 (COVID-19) and associated health risks**

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## Text S1 Quantification of the use rates of disinfecting chemicals

The “surface application” scenario:  $U = S_{\text{surface}} \cdot AL \cdot C$ , and

The “hand hygiene” scenario:  $U = AM \cdot C$ .

whereby,

$S_{\text{surface}}$ : Area of the disinfected hard surfaces (in  $\text{m}^2$ ). We assume that  $S_{\text{hard}}$  follows the normal distribution, with a mean (central tendency) of  $3 \text{ m}^2$  in each home taken from McCready et al. (2013) and a relative standard deviation of 30% considering the variation in the floor area of a home (based on the mean and standard deviation of “the area of the first floor” in houses recorded in the U.S. Residential Energy Consumption Survey database). The normal distribution is selected because it approximates the surveyed distribution in the area of the first floor (with a skewness of 0.58 close to 0 for the normal distribution, and a kurtosis of 4.30 close to 3 for the normal distribution).

$AL$ : Area-specific application load of disinfectant product per use (in  $\text{g}/\text{m}^2$ ). We assume that  $AL$  follows a normal distribution with a mean of  $8.70 \text{ g}/\text{m}^2$  and a standard deviation of  $0.32 \text{ g}/\text{m}^2$ , which is derived based on experimental data that cleaning a  $3868 \pm 108 \text{ cm}^2$  kitchen sink consumes  $3.37 \pm 0.077 \text{ g}$  of “wet fraction” in wet wipes (Weerdesteijn et al. 1999).

$AM$ : Amount of disinfectant product per use (in g). We follow the assumption in Sanderson et al. (2006) that  $AL_{\text{surface}}$  follows a uniform distribution ranging from 1.6 to 1.7 g (internal data from the Soap and Detergent Association).

$C$ : Weight fraction of active ingredient (in %). A search of the U.S. EPA’s Chemicals and Products Database (CPDat) (Dionisio et al. 2018) (available through the U.S. EPA’s CompTox Chemistry Dashboard) indicates that the weight fraction of a disinfecting chemical varies by up to three orders of magnitude between specific disinfecting products and that there is considerable overlap between the weight fractions of different disinfecting chemicals. For instance, available records show that the reported weight fraction of a benzalkonium chloride mixture (CASRN 8001-54-5; DTXSID 9034317) ranges from 0.38% in antibacterial hand soaps and sprays to 17.4% in multi-purpose sprays, whereas that of triclosan (CASRN 3380-34-5; DTXSID 5032498) ranges from 0.1% to 7% in antibacterial hand soaps. It should be noted that product-specific records of weight fraction are incomplete in CPDat: records are missing for several disinfecting chemicals investigated in our work (see the list in Section 2.3) or their certain types of disinfecting products. As such, instead of collecting reported weight fractions for individual specific chemical-product combinations, we use an estimate pooling weight fractions of all the investigated disinfecting chemicals in the “product category” of cleaning products predicted by Isaacs et al. (2018), which ranges from the 5<sup>th</sup> percentile of 0.0071% to the 95<sup>th</sup> percentile of 9.3%, with a median of 1.8%. We assume that it follows a triangular distribution. We do not consider the dilution of disinfectants during use.

**Text S2** Inhalation exposure during the spraying of disinfecting products

The inhalation exposure during the spraying of disinfecting products is estimated to be 67 ng/kg/d (the worst case) by the spray module (for non-volatile substances) in ConsExpo (web version 1.0.7, last update: March 31, 2020). This rough estimation assumes exposure duration to be 10 min, which is the maximum “contact time”, i.e., the duration that a disinfecting chemical is in contact with the novel coronavirus (SARS-CoV-2) to achieve complete inactivation, recommended by the U.S. Environmental Protection Agency for disinfecting products (U.S. Environmental Protection Agency 2020). The inhalation rate is assumed to be 25 L/min (a default in ConsExpo). We assume an instantaneous release of disinfectants. Other parameters are the same as those used in the PROTEX simulation.

**Table S1** Properties of the active ingredients (neutral forms) in disinfecting products against COVID-19

Chemical	CAS#	Molar mass (g/mol) <sup>a</sup>	logK <sub>OW</sub> <sup>b</sup>	logK <sub>AW</sub> <sup>c</sup>	pK <sub>a</sub> <sup>d</sup>	OH reaction rate constant (cm <sup>3</sup> /molecule/s) <sup>e</sup>	log V <sub>P</sub> (Pa) <sup>f</sup>	log S <sub>w</sub> (mol/L) <sup>g</sup>	log HL <sub>B</sub> (hour) <sup>h</sup>
C8BAC	959-55-7	283.88 (248.24)	0.504	-3.5		2.50E-11	-1.66	-4.55	0.87 (0.18)
C10BAC	965-32-2	311.94 (276.27)	1.802	-4.58		2.63E-11	-2.58	-4.39 <sup>i</sup>	0.82 (0.19)
C12BAC	139-07-1	339.99 (304.30)	2.62 <sup>j</sup>	-10.68		3.04E-11	-6.46 <sup>k</sup>	-2.17 <sup>l</sup>	0.77 (0.2)
C14BAC	139-08-2	368.05 (332.33)	3.14 <sup>m</sup>	-6.68		3.58E-11	-3.74 <sup>n</sup>	-3.45 <sup>o</sup>	0.74 (0.21)
C16BAC	122-18-9	396.1 (360.36)	3.02 <sup>p</sup>	-8.13		3.74E-11	-3.63	-1.89 <sup>q</sup>	0.71 (0.22)
C18BAC	122-19-0	424.15 (388.39)	3.36 <sup>r</sup>	-6.95		3.89E-11	-4.81	-4.25 <sup>s</sup>	0.69 (0.23)
C12ADEAC	14351-42-9	368.05 (332.33)	3.032	-4.38		3.56E-11	-3.76	-5.77	0.85 (0.21)
C14ADEAC	27479-29-4	396.1 (360.36)	3.7	-4.28		3.71E-11	-3.92	-6.03	0.82 (0.22)
DODAC	5538-94-3	305.98 (270.32)	2.353	-5.99		2.36E-11	-2.69 <sup>t</sup>	-3.09 <sup>u</sup>	0.9 (0.32)
DDDAC	7173-51-5	362.08 (326.38)	2.53 <sup>v</sup>	-5.64		2.60E-11	-2.22 <sup>w</sup>	-2.97 <sup>x</sup>	0.84 (0.32)
ODDAC	32426-11-2	334.03 (298.35)	2.781	-2.96		2.5E-11	-2.59	-6.025	0.87 (0.32)
C14ADBAS	68989-01-5	514.8 (332.33)	3.02	-4.21		3.58E-11	-3.35	-5.53	0.74 (0.21)
Benzethonium Chloride	121-54-0	448.09 (412.32)	1.02 <sup>y</sup>	-13.58		6.21E-11	-7.56 <sup>z</sup>	-0.37 <sup>aa</sup>	0.91 (0.14)
Cetrimonium Bromide	57-09-0	364.456 (284.33)	2.66	-7.85		2.03E-11	-2.22	-0.76 <sup>ab</sup>	0.9 (0.32)
Chloroxylonol	88-04-0	156.61	3.27 <sup>ac</sup>	-3.66	9.7 <sup>ad</sup>	7.11E-11	0.03	-2.7 <sup>ac</sup>	0.58 (0.16)
Thymol	89-83-8	150.221	3.30 <sup>af</sup>	-4.75	10.62 <sup>ag</sup>	9.4E-11	-0.53 <sup>ah</sup>	-2.175 <sup>ai</sup>	0.83 (0.11)
O-Phenylphenol	90-43-7	170.211	3.12 <sup>aj</sup>	-4.3	10	5.58E-11	-0.31 <sup>ak</sup>	-2.405 <sup>al</sup>	0.63 (0.1)
Triethylene glycol	112-27-6	150.174	-1.75 <sup>am</sup>	-8.18	14.06	3.26E-11	-0.97 <sup>an</sup>	0.82 <sup>ao</sup>	-0.04 (0.23)
Bronopol	52-51-7	199.988	0.47	-9.34	12.02	2.07E-12	-2.77 <sup>ap</sup>	0.175 <sup>aq</sup>	0.05 (0.15)
Chlorhexidine Gluconate	18472-51-0	897.76 (504.20)	-1.86 <sup>ar</sup>	-8.66	11.51 <sup>as</sup>	1.67E-10	-2.29 <sup>at</sup>	-0.02 <sup>au</sup>	1.51 (0.15)
Triclocarban	101-20-2	315.58	3.63 <sup>av</sup>	-6.61	12.7 <sup>aw</sup>	1.66E-11	-5.92	-5.7 <sup>ax</sup>	2.13 (0.08)
Triclosan	3380-34-5	289.54	4.8 <sup>ay</sup>	-5.89	7.9 <sup>az</sup>	1.68E-11	-3.99	-4.495 <sup>ba</sup>	2.05 (0.09)

## Notes

- a) Molar mass in g/mol; in brackets are the molar mass of the parent compound without counterion.
- b) Predicted using the ACD/Labs Consensus Model unless indicated if experimentally determined values are available.
- c) Calculated from  $V_p$  and  $S_w$ :  $K_{AW} = V_p/(S_w * R * T)$ , where  $T$  is the temperature (298.15 K) and  $R$  is the ideal gas constant (8314.463 Pa L mol<sup>-1</sup> K<sup>-1</sup>).
- d) Predicted using ACD/Labs unless indicated if experimentally determined values are available.
- e) Consensus of EPI Suite<sup>TM</sup> and OPERA predictions.
- f) Consensus of NICEATM and OPERA predictions.
- g) Consensus of NICEATM and OPERA predictions.
- h) Predicted using the biotransformation model published in Papa et al. (2018) and implemented in QSARINS-Chem (Gramatica et al. 2014); in brackets are the 95% confidence intervals of the predictions.
- i) Converted from an experimentally determined value of  $\geq 10$  mg/ml ( $\log S_w = -4.49$  mol/L) at 63 °F (17.2 °C) according to the National Toxicology Program in the PubChem database.
- j) Converted from an experimentally determined value at 24 °C, determined using shake flask method according to the OECD Guideline 107 and EU Method A.8 reported and in the Registered Substances Dossier by the European Chemical Agency (ECHA) (European Chemical Agency 2020).
- k) Experimental value at 25 °C, determined using the Knudsen cell effusion method according to OECD Guideline 104 and EU Method A.4 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- l) Converted from an experimentally determined value of  $> 2000$  mg/L ( $\log S_w = -2.23$  mol/L) at 20 °C, determined using the preliminary solubility test method as part of the partition coefficient test according to the OECD 107 as well as using the CMC method, according to ISO 4311 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- m) Converted from an experimentally determined value of  $\log K_{ow} = 3.20$  at 20 °C, determined using shake flask method according to the OECD Guideline 107 and EU Method A.8 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- n) Experimental value at 25 °C, determined using the vapor pressure balance method according to OECD Guideline 104 and EU Method A.4 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- o) Converted from an experimentally determined value of 115 mg/L ( $\log S_w = -3.51$  mol/L) at 20 °C, determined using the flask method according to the OECD Guideline 105 and EU Method A.6 as well as using the CMC method according to ISO 431 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- p) Experimental value at 25 °C (pH 5.8), determined using the reverse phase high-performance liquid chromatography method according to OECD Guideline 117 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- q) Experimental value at 25 °C, determined using the spectrophotometric analytical method according to the OECD Guideline 105 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- r) Arithmetic mean of experimental values reported by Hansch et al. (1985) ( $\log K_{ow} = 3.23$  at 25 °C), and by ECHA (European Chemical Agency 2020) in the Registered Substances Dossier ( $\log K_{ow} = 3.89$  at 20 °C) and Hodges et al. (2019) ( $\log K_{ow} = 3.03$  at 25 °C). The value measured using a slow-stirring method by Hodges et al. (2019) is excluded because “the values determined using the slow-stirring method seem lower than would be expected,

particularly given the size of the longer alkyl chain molecules".(Hodges et al. 2019)

- s) Converted from an experimentally determined value of 20.8 mg/L ( $\log S_w = -4.31$  mol/L) at 20 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- t) Experimental value at 25 °C, determined using the effusion method based on vapor pressure balance according to OECD Guideline 104 and EU Method A.4 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- u) Experimental value of the critical micelle concentration at 25 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- v) Converted from an experimentally determined value of  $\log K_{ow} = 2.59$  at 20 °C, derived as the ratio of the solubility in octanol (250 g/L) to that in water (0.65 g/L; critical micelle concentration) and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- w) Experimental value at 25 °C, determined using the isothermal thermogravimetric effusion method according to OECD Guideline 104 and EU method A.4 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- x) Experimental value of the critical micelle concentration at 25 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- y) Converted from an experimentally determined value  $\log K_{ow} = 1.08$  at 20 °C, determined using the shake-flask method according to the OECD Guideline 107 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- z) Experimental value at 25 °C, determined using the vapor pressure balance method according to OECD Guideline 104 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- aa) Arithmetic mean of experimental values: (i)  $\log S_w = 0.13$  mol/L at 25 °C based on a measurement of 530 g/L at 20 °C determined using the modified flask method according to OECD 105 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020) and (ii)  $\log S_w = -0.87$  mol/L at 25 °C based on a measurement of 50 mg/mL at 64° F reported by the National Toxicology Program in the PubChem database.
- ab) Converted from an experimentally determined value of 55 g/L at 20 °C measured by a simple water solubility test and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- ac) Experimental value at 25 °C reported by Sangster (2019).
- ad) Taken from Kortum et al. (1961).
- ae) Arithmetic mean of two values at 20 °C (i)  $\log S_w = -2.72$  mol/L, based on measurements of 0.3 g/L (pH 4 and 7) and 0.8 g/L (pH 10) as reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020), and (ii)  $\log S_w = -2.79$  mol/L by Yalkowsky et al. (2003)
- af) Experimental value at 25 °C reported by Hansch et al. (1985).
- ag) Experimental value at 20 °C as reported by Serjeant and Dempsey (1979).
- ah) Experimental values at 25 °C reported by Jones (1960).
- ai) Arithmetic mean of two experimental values: (i)  $\log SW = -2.16$  mol/L at 25 °C based on a value of 900 mg/L at 20 °C reported by Yalkowsky and Dannenfelser (1992) (ii)  $\log SW = -2.19$  mol/L based on a reported value of 980 mg/L at 25 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- aj) Arithmetic mean of experimental values reported by Hansch et al. (1985) ( $\log K_{ow} = 3.09$  at 25 °C) and by ECHA (European Chemical Agency 2020) in the Registered Substances Dossier ( $\log K_{ow} = 3.15$  at 25 °C converted from a value of 3.18 at 22.5 °C determined by the shake-flask method according to EU Method A.8).

- ak) Arithmetic mean of experimental values at 25 °C (i)  $\log V_p = -0.57$  Pa ( $V_p = 0.267$  Pa) reported by Kundel (1975) and (ii)  $\log V_p = -0.04$  Pa ( $V_p = 0.906$  Pa) determined by effusion method according to EU Method A.4 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- al) Arithmetic mean of two experimental values (i)  $\log W_s = -2.39$  mol/L ( $W_s = 700$  mg/L) at 25 °C reported by Tomlin (2004) and (ii)  $\log W_s = -2.42$  mol/L at 25 °C converted from a value of 0.56 g/L at 20 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- am) Experimental value at 25 °C reported by Meylan and Howard (1995).
- an) Geometric mean of two values at ~25 °C (i) 0.000655 hPa reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020) and (ii) 0.00132 mmHg by Daubert and Danner (1989).
- ao) Experimental value at 25 °C reported by Riddick et al. (1986).
- ap) Converted from an experimentally determined value  $V_p = 1.68 \times 10^{-3}$  Pa at 20 °C (Tomlin 2004).
- aq) Arithmetic mean of two experimental values (i)  $\log W_s = 0.13$  at 25 °C converted from a value of 255000 mg/L at 22 °C reported by Yalkowsky et al. (2003) and (ii)  $\log W_s = 0.22$  at 25 °C converted from a value of 286 g/L at 20 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- ar) Converted from the experimental value of  $\log K_{ow} = -1.81$  at 20.7 °C determined by the Shake Flask Method reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- as) pKa of the base predicted by ACD/Labs
- at) Experimental value at 25 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- au) Converted from a value of  $W_s = 750$  g/L at 20 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- av) Experimental value at 25 °C determined by using reverse phase high-performance liquid chromatographic method according to OECD Guideline No. 117 reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- aw) Experimental value as reported by Wu et al. (2009).
- ax) Experimental value at 25 °C measured by the spectrophotometric analytical method as per OECD 101 and reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- ay) Arithmetic mean of two experimental values (i)  $\log K_{ow} = 4.76$  at 25 °C reported by the Chemicals Inspection And Testing Institute (Chemicals Inspection and Testing Institute 1992) and (ii)  $\log K_{ow} = 4.84$  at 25 °C converted from a  $\log K_{ow} = 4.9$  at 20 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).
- az) Experimental value reported by O'Neil and Heckelman (2013).
- ba) Arithmetic mean between two values (i)  $\log W_s = -4.4$  at 25 °C Converted from an experimentally determined value of 10 mg/L at 20 °C reported by Yalkowsky and Dannenfelser (1992) and (ii)  $\log W_s = -4.59$  at 25 °C Converted from an experimentally determined value of 6.5 mg/L at 20 °C reported in the Registered Substances Dossier by ECHA (European Chemical Agency 2020).



**Table S2** Modeled exposures to DODAC and *O*-phenylphenol assuming their lifetimes in organic films are 240 and 9200 days, relative to the default assumption of no degradation (= 100%).

N.B.: There is no difference between age groups.

	DODAC	<i>O</i> -phenylphenol
240 days	16%	93%
9200 days	88%	99%
Default assumption (no degradation)	100%	100%

**Table S3** Summary of *in vivo* toxicological data from the U.S. EPA's CompTox Chemistry Dashboard and European Chemicals Agency

Chemicals	CAS#	RfD (mg/kg/day)	DNEL (mg/kg/day)		Hazard
			General population	Worker	
C8BAC	959-55-7	NA	NA		
C10BAC	965-32-2	NA	NA		
C12BAC	139-07-1	NA	No hazard identified		
C14BAC	139-08-2	NA	No hazard identified		
C16BAC	122-18-9	NA	NA		
C18BAC	122-19-0	NA	No hazard identified		
C12ADEAC	14351-42-9	NA	NA		
C14ADEAC	27479-29-4	NA	NA		
DODAC	5538-94-3	NA	1.6	2.67	Irritation
DDDAC	7173-51-5	0.1	No hazard identified	8.6	Irritation; decreased total cholesterol level
ODDAC	32426-11-2	NA	NA		
C14ADBAS	68989-01-5	NA	NA		
Chloroxylenol	88-04-0	NA	Low hazard	5	Skin sensitization
Triethylene glycol	112-27-6	2	No hazard identified		Delayed ossification of the supraoccipital bone in fetal mice
Benzethonium Chloride	121-54-0	NA	NA		
Cetrimonium Bromide	57-09-0	NA	Hazard unknown	0.4	Irritation
Bronopol	52-51-7	NA	0.7	2	Irritation
Chlorhexidine Gluconate	18472-51-0	NA	3	5	Irritation
Chlorhexidine	55-56-1	NA	NA		
Thymol	89-83-8	NA	8.3	16.6	Histopathological changes in the forestomach
O-Phenylphenol	90-43-7	NA	0.4	21.84	Irritation
Triclocarban	101-20-2	NA	0.25	0.7	Low hazard
Triclosan	3380-34-5	0.3 - 4	No hazard identified	2.8	Irritation; hepatocellular hypertrophy; effect on the lining of stomach

**Table S4** Summary of *in vitro* bioactivity data from ToxCast

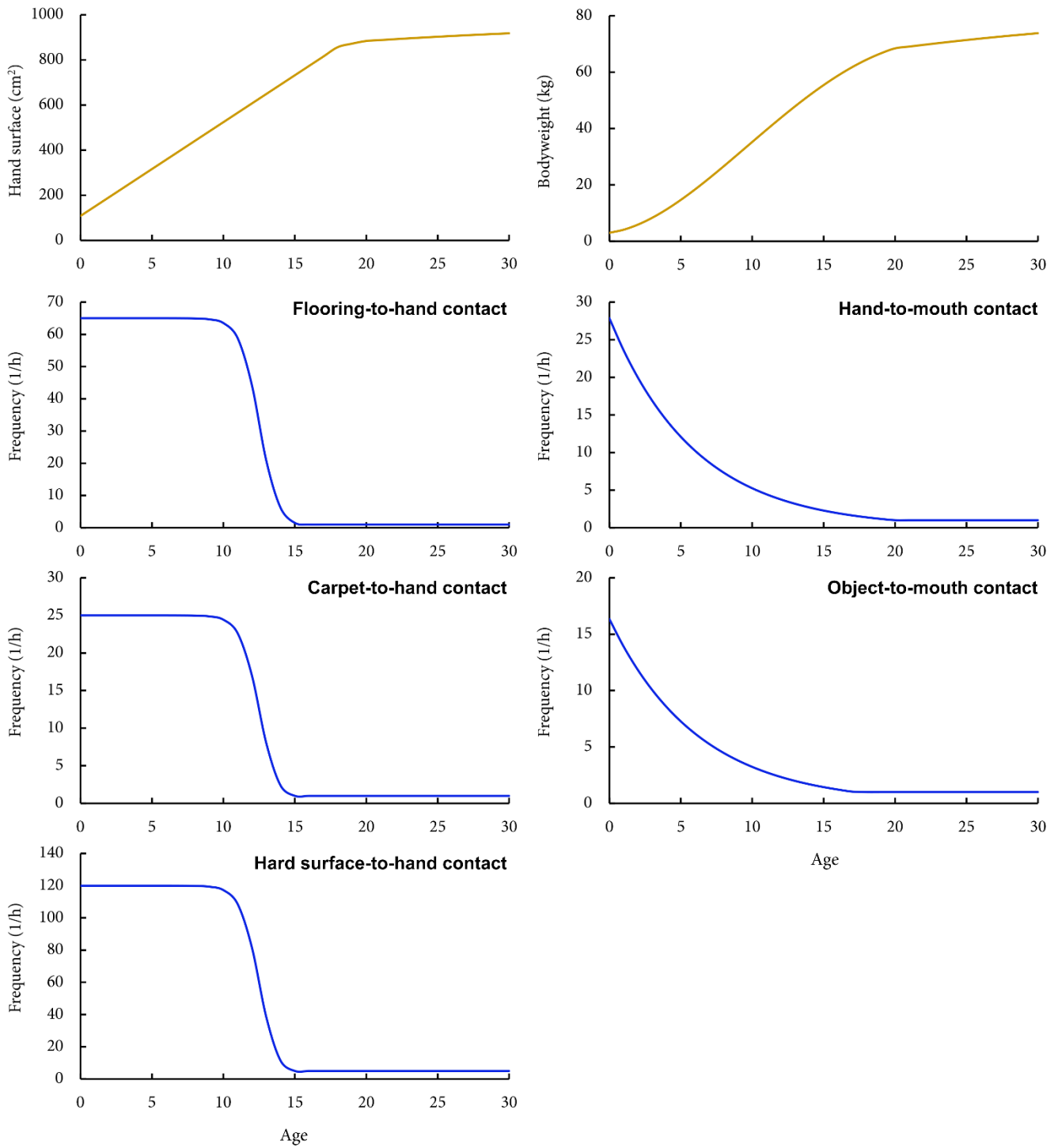
Chemicals	CAS#	Number of active assays	Bioactivity (uM)							Targets of active assay with AC <sub>50</sub> below cytotoxicity limit
			Cytotoxicity		AC <sub>50</sub>					
			Center	Limit	5th	25th	50th	75th	95th	
C8BAC	959-55-7	0	NA							
C10BAC	965-32-2	0	NA							
C12BAC	139-07-1	142	35.05	7.33	0.29	0.46	1.88	3.98	6.405	Cell cycle; DNA binding; Nuclear receptor
C14BAC	139-08-2	0	NA							
C16BAC <sup>a</sup>	122-18-9	251	25.3	4.72	0.5272	2	3.22	4	4	Cell adhesion molecules; Cell cycle; Cell morphology; Cytochromes P450; Cytokinetics; DNA binding; G protein-coupled receptor; Ion channel; Kinase; Misc. protein; Oxidoreductase; Phosphatase; Protease; Protease inhibitor; Transporter
C18BAC <sup>a</sup>	122-19-0	245	30.3	6.07	0.2	0.7	1.28	2	4.148	Cell adhesion molecules; Cell cycle; Cell morphology; Cytochromes P450; Cytokinetics; DNA binding; G protein-coupled receptor; Growth factor; Kinase; Misc. protein; Phosphatase; Protease; Protease inhibitor; Transporter;
C12ADEAC	14351-42-9	0	NA							
C14ADEAC	27479-29-4	0	NA							
DODAC	5538-94-3	20	19.6	4.28	0.6676	0.766	0.889	1.0295	1.1419	Cell cycle
DDDAC	7173-51-5	327	29.7	5.2	1.0345	3.9175	4	4	4.637	Cell adhesion molecules; Cell cycle; Cell morphology; Cytochromes P450; DNA binding; G protein-coupled receptor; Growth factor; Ion channel; Kinase; Malformation; Misc. protein; Nuclear receptor; Protease; Protease inhibitor; Transporter
ODDAC	32426-11-2	0	NA							
C14ADBAS	68989-01-5	0	NA							
Chloroxylenol	88-04-0	43	7.625	1.66	NA					
Triethylene glycol	112-27-6	15	0.00129	0	NA					
Benzethonium	121-54-0	235	5.48	26	0.04	0.25	2.39	3.305	4.63	Cell adhesion molecules; Cell cycle; Cytochromes P450;

Chloride										Cytokinetics; DNA binding; Esterase; G protein-coupled receptor; Growth factor; Ion channel; Misc. protein; Nuclear receptor; Protease; Steroid hormone; Transporter;
Cetrimonium Bromide	57-09-0	186	6.74	29.25	0.78125	1.58	3.415	5.1675	6.5175	Cell cycle; DNA binding; Nuclear receptor
Bronopol	52-51-7	185	11.08	57.5	1.397	4.08	9.72	10	10	Cell adhesion molecules; Cell cycle; Cytochromes P450; Cytokinetics; DNA binding; G protein-coupled receptor; Kinase
Chlorhexidine Gluconate	18472-51-0	0	NA							
Chlorhexidine	55-56-1	144	6.32	29.15	2.35	2.64	3.89	5	6.024	Cell cycle; DNA binding; Nuclear receptor
Thymol <sup>a</sup>	89-83-8	21	47.2	12.3	3.277	6.27	10	10	10	Cell morphology; Cytokinetics; G protein-coupled receptor
O-Phenylphenol <sup>a</sup>	90-43-7	91	41.65	9.21	3.536	3.76	4.04	4.33	4.562	Cell cycle; Cytochromes P450
Triclocarban <sup>a</sup>	101-20-2	186	4.93	1	0.162715	0.34	0.48	0.626	0.7948	Cell cycle; Cell morphology; Esterase; Nuclear receptor; Steroid hormone
Triclosan	3380-34-5	321	35.4	7.34	1.406	2.45	4.62	5.2775	6.793	Cell adhesion molecules; Cell cycle; Cell morphology; Cytochromes P450; Cytokinetics; DNA binding; G protein-coupled receptor; Kinase; Malformation; Nuclear receptor; Transporter

### Notes

a) More than half of the active assays with AC<sub>50</sub> lower than cytotoxicity limit have notation indicating original data being noisy.

**Figure S1** Age-dependent evolution of hand surface area, bodyweight, frequencies of hand contact with surfaces (flooring, carpet, and hard surfaces), and frequencies of mouthing hands and objects

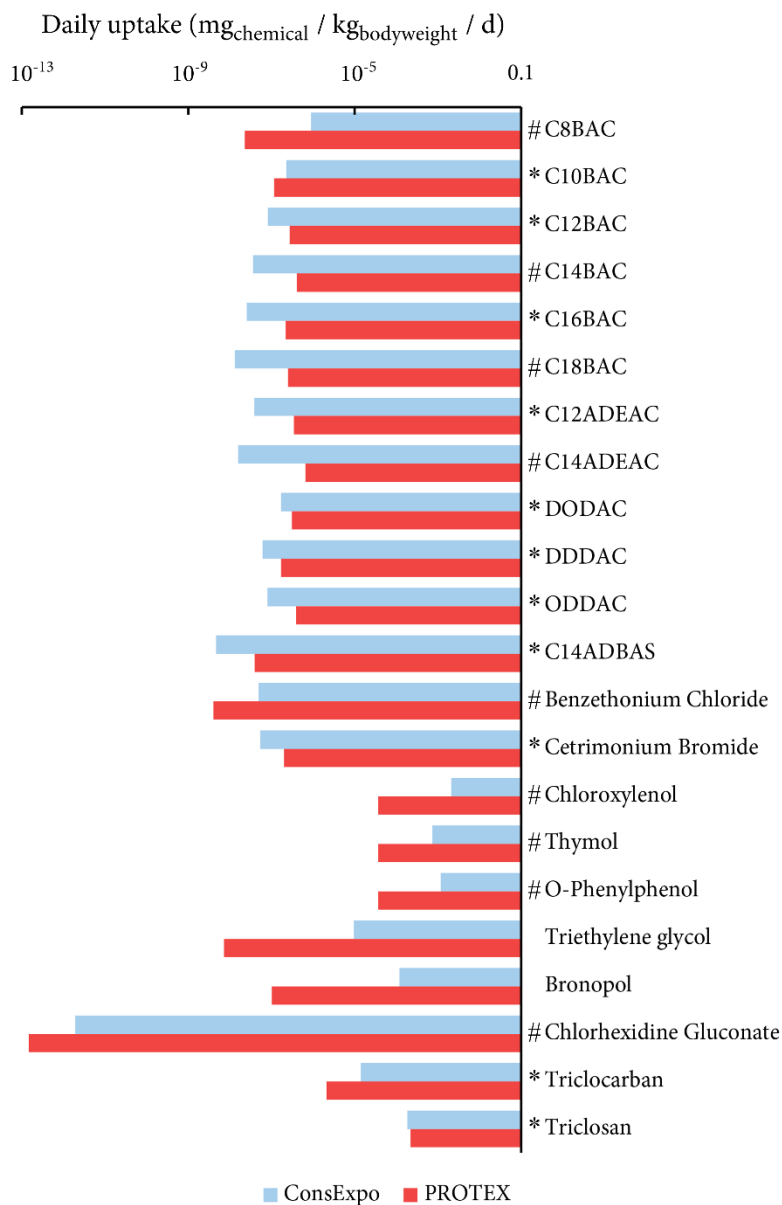


Note: The surface area of two hands is assumed to be 5% of the total body area calculated according to the literature (Haycock et al. 1978; Mosteller 1987). The age-dependence of bodyweight is obtained by fitting

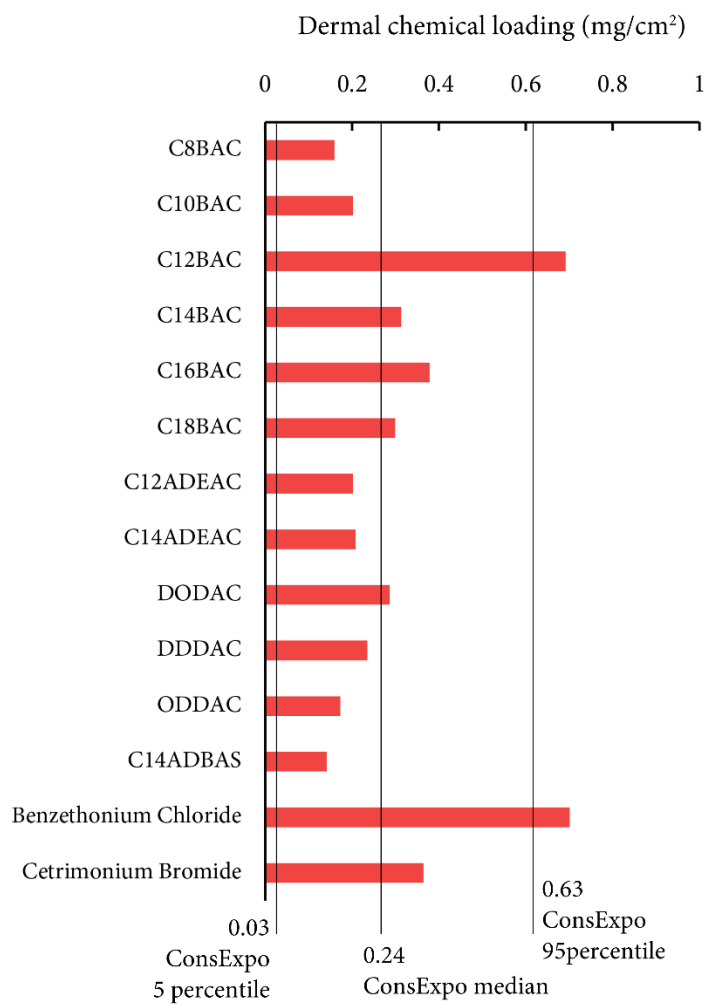
nationally surveyed data in the U.S. EPA's Exposure Factors Handbook (U.S. Environmental Protection Agency 2019). Frequencies of hand contacts with flooring, carpet, and hard surfaces are taken from Freeman et al. (2001)(for children) and Zhang et al. (2014)(for adults). Frequencies of hand-to-mouth and object-to-mouth contacts are obtained by fitting recommended observed data in the U.S. EPA's Exposure Factors Handbook (U.S. Environmental Protection Agency 2019).

**Figure S2** Comparison between PROTEX and ConsExpo predictions of dermal uptake of disinfecting chemicals during 20-s hand washing each day in the “hand hygiene” scenario

“\*” marks chemicals with a difference between PROTEX and ConsExpo predictions within an order of magnitude; “#” marks chemicals with a difference between PROTEX and ConsExpo predictions within an order of magnitude

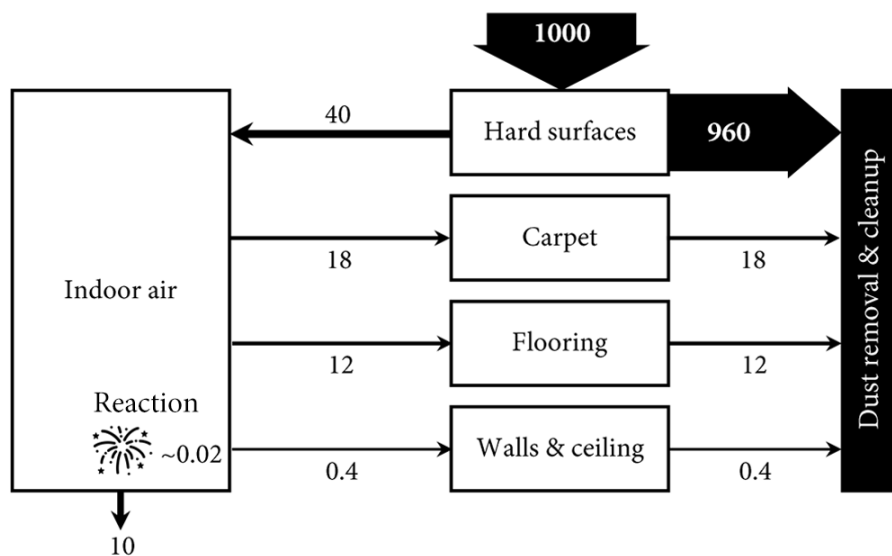


**Figure S3** Comparison between PROTEX and ConsExpo predictions of dermal loadings of quaternary ammonium salts on hands in the “surface application” scenario

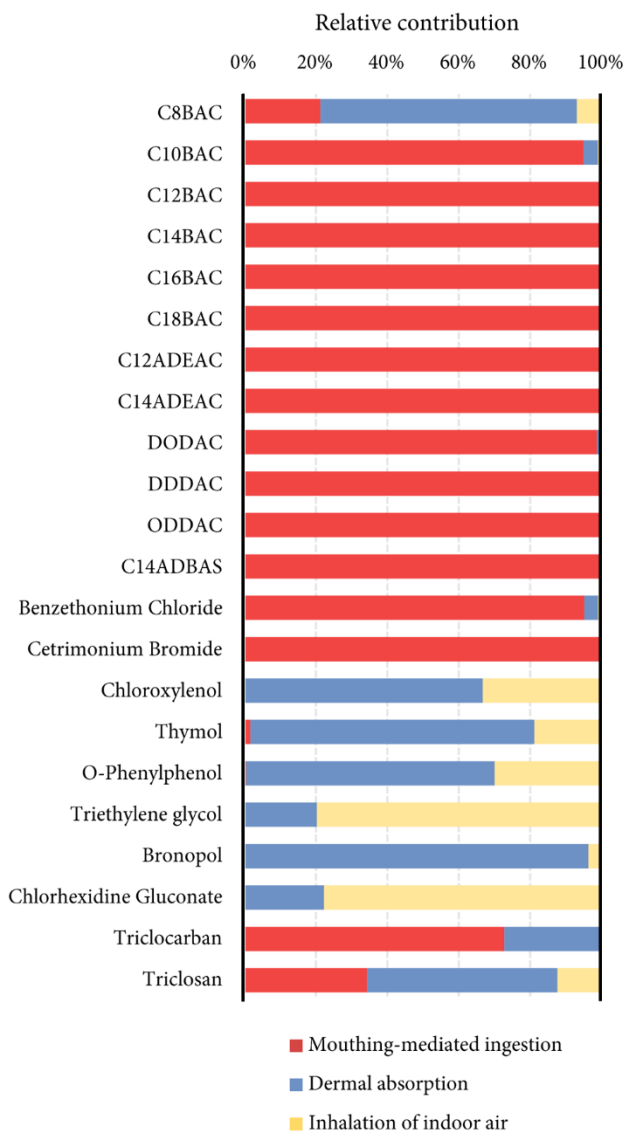




**Figure S4** Fate and transport of neutral dioctyl dimethyl ammonium chloride (DODAC) between indoor compartments, assuming no dissociation (ionization) of DODAC



**Figure S5** Relative contribution of mouthing-mediated ingestion, dermal absorption, and inhalation of indoor air to aggregate exposure of the modeled 25-year-old child to disinfecting chemicals



## References

- Chemicals Inspection and Testing Institute. Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo: National Institute of Technology and Evaluation; 1992
- Daubert, T.E.; Danner, R.P. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis; 1989
- Dionisio, K.L.; Phillips, K.; Price, P.S.; Grulke, C.M.; Williams, A.; Biryol, D.; Hong, T.; Isaacs, K.K. The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products. *Scientific Data*. 5:180125; 2018
- European Chemical Agency. Registered Substances Database (<https://echa.europa.eu/information-on-chemicals/registered-substances>). Helsinki: European Chemical Agency (ECHA) (accessed May 25, 2020); 2020
- Freeman, N.; Jimenez, M.; Reed, K.; Gurunathan, S.; Edwards, R.; Roy, A.; Adgate, J.; Pellizzari, E.; Quackenboss, J.; Sexton, K. Quantitative analysis of children's microactivity patterns: The Minnesota Children's Pesticide Exposure Study. *J Expo Sci Environ Epidemiol*. 11:501-509; 2001
- Gramatica, P.; Cassani, S.; Chirico, N. QSARINS-chem: Insubria datasets and new QSAR/QSPR models for environmental pollutants in QSARINS. *J Comput Chem*. 35:1036-1044; 2014
- Hansch, C.; Leo, A.; Hoekman, D.H. Exploring QSAR: Hydrophobic, Electronic, and Steric Constants. Washington D.C.: American Chemical Society; 1985
- Haycock, G.B.; Schwartz, G.J.; Wisotsky, D.H. Geometric method for measuring body surface area: A height-weight formula validated in infants, children, and adults. *J Pediatr*. 93:62-66; 1978
- Hodges, G.; Eadsforth, C.; Bossuyt, B.; Bouvy, A.; Enrici, M.H.; Geurts, M.; Kotthoff, M.; Michie, E.; Miller, D.; Muller, J.; Oetter, G.; Roberts, J.; Schowanek, D.; Sun, P.; Venzmer, J. A comparison of log K<sub>ow</sub> (n-octanol-water partition coefficient) values for non-ionic, anionic, cationic and amphoteric surfactants determined using predictions and experimental methods. *Environ Sci Eur*. 31; 2019
- Isaacs, K.K.; Phillips, K.A.; Biryol, D.; Dionisio, K.L.; Price, P.S. Consumer product chemical weight fractions from ingredient lists. *J Expo Sci Environ Epidemiol*. 28:216-222; 2018
- Jones, A. Sublimation pressure data for organic compounds. *J Chem Eng Data*. 5:196-200; 1960
- Kortum, G.; Vogel, W.; Andrussov, K. Dissociation Constants of Organic Acids in Aqueous Solution. London: Butterworth & Co. Ltd.; 1961
- Kundel, H. Determination of the saturated vapor pressure for alkyl resorcinols and their methyl ethers. *Tr Tallin Politekh Inst*. 390:107-115; 1975
- McCready, D.; Pitt, J.; Fontaine, D.D.; Busby, M.I. Potential sequential exposures to 2-butoxyethanol after use of a hard-surface cleaner. *Hum Ecol Risk Assess*. 19:189-214; 2013
- Meylan, W.M.; Howard, P.H. Atom/fragment contribution method for estimating octanol-water partition coefficients. *J Pharm Sci*. 84:83-92; 1995
- Mosteller, R.D. Simplified calculation of body-surface area. *N Engl J Med*. 317:1098; 1987
- O'Neil, M.J.; Heckelman, P.E. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, U.K.: Royal Society of Chemistry; 2013
- Papa, E.; Sangion, A.; Arnot, J.A.; Gramatica, P. Development of human biotransformation QSARs and application for PBT assessment refinement. *Food Chem Toxicol*. 112:535-543; 2018

- Riddick, J.A.; Bunger, W.B.; Sakano, T.K. *Organic Solvents: Physical Properties and Methods of Purification*. 4th Edition. New York: Wiley-Interscience; 1986
- Sanderson, H.; Counts, J.L.; Stanton, K.L.; Sedlak, R.I. Exposure and prioritization - Human screening data and methods for high production volume chemicals in consumer products: Amine oxides a case study. *Risk Anal.* 26:1637-1657; 2006
- Sangster, J. LOGKOW Database. A databank of evaluated octanol-water partition coefficients (Log P). Montreal, Quebec: Sangster Research Laboratories 2019
- Serjeant, E.P.; Dempsey, B. *Ionisation Constants of Organic Acids in Aqueous Solution*. Oxford and New York: Pergamon Press; 1979
- Tomlin, C.D.S. *The e-Pesticides Manual (Version 3.0)*; 13th Ed. Hampshire: British Crop Protection Council; 2004
- U.S. Environmental Protection Agency. *Exposure Factors Handbook (2011 Edition; 2019 Update)*. Washington, D.C.: National Center for Environmental Assessment, Office of Research and Development; 2019
- U.S. Environmental Protection Agency. List N: Disinfectants for Use Against SARS-CoV-2 (COVID-19) (available at: <https://cfpub.epa.gov/giwiz/disinfectants/index.cfm>). Washington, D.C.: U.S. Environmental Protection Agency; 2020
- Weerdesteijn, M.C.H.; Bremmer, H.J.; Zeilmaker, M.J.; van Veen, M.P. *Hygienic Cleaning Products Used in the Kitchen: Exposure and Risks (RIVM report 612810008)*. Bilthoven, The Netherlands; 1999
- Wu, C.; Spongberg, A.L.; Witter, J.D. Adsorption and degradation of triclosan and triclocarban in soils and biosolids-amended soils. *J Agric Food Chem.* 57:4900-4905; 2009
- Yalkowsky, S.H.; Dannenfelser, R.M. *Aquasol Database of Aqueous Solubility*. Tucson, AZ: College of Pharmacy, University of Arizona; 1992
- Yalkowsky, S.H.; He, Y.; Jain, P. *Handbook of Aqueous Solubility Data*. Boca Raton, FL: CRC Press; 2003
- Zhang, X.; Arnot, J.A.; Wania, F. Model for screening-level assessment of near-field human exposure to neutral organic chemicals released indoors. *Environ Sci Technol.* 48:12312-12319; 2014