Chemical name	CASRN	Water Flea[b]	Fathead Minnow[c]	Rainbow Trout[d]	Green Algae[e]	Frequency of use (% events)	Median mass per event (kg)
1,2,3-Trimethylbenzene	526-73-8	-	-	-	2	0.3%	1.0
1,2,4-Trimethylbenzene	95-63-6	2	2	-	2	5.7%	1.6
1,3,5-Trimethylbenzene	108-67-8	2	-	-	2	0.3%	2.3
2-Mercaptoethyl alcohol	60-24-2	2	-	-	2	0.7%	2.5
2-Methyl-3(2H)-isothiazolone	2682-20-4	1	-	1	1	0.2%	2.6
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	1	-	1	1	0.1%	5.2
Acrylamide	79-06-1	3	>3	>3	1	0.8%	<0.1
Alcohols, C10-14, ethoxylated	66455-15-0	-	-	-	1	0.6%	64
Aluminum	7429-90-5	-	-	1	-	16.5%	9.1
Ammonium chloride	12125-02-9	>3	2	>3	-	48.4%	454
Benzene, c10-c16 alkyl derivatives	68648-87-3	-	-	-	1	0.9%	<0.1
Benzene, tetrapropylene-	25265-78-5	-	-	-	1	0.1%	2.7
Benzoisothiazolinone	2634-33-5	1	-	1	1	0.1%	<0.1
Bis(isopropyl)naphthalene	38640-62-9	-	-	-	1	2.0%	1.8
Canola oil	120962-03-0	-	-	-	1	0.3%	92
Cocamidopropyl betaine	61789-40-0	2	-	-	>3	0.7%	<0.1
Cyclohexasiloxane, 2,2,4,4,6,6,8,8,10,10,12,12-dodecamethyl-	540-97-6	-	-	-	1	0.3%	<0.1
Cyclopentasiloxane, 2,2,4,4,6,6,8,8,10,10-decamethyl-	541-02-6	-	-	-	1	0.3%	<0.1
DBNPA (2,2-dibromo-3-nitrilopropionamide)	10222-01-2	1	1	1	1	0.3%	4.1
Dodecylbenzene	123-01-3	-	-	-	1	0.1%	5.4
Dodecylbenzene sulfonic acid	27176-87-0	2	-	2	3	1.4%	<0.1
Ethanesulfonic acid, 2-[methyl[(9z)-1-oxo-9-octadecen-1-yl]amino]-, sodium salt (1:1)	137-20-2	-	-	-	2	0.6%	53
Ethoxylated C14-15 alcohols	68951-67-7	1	1	1	1	1.3%	2.4
Ethoxylated hexanol	68439-45-2	2	-	2	>3	0.3%	16
Ethylbenzene	100-41-4	2	2	2	2	31.3%	2.9
Fatty acids, tall-oil	61790-12-3	>3	-	-	1	0.4%	7.1
Fatty acids, tall-oil, reaction products with triethanolamine	67784-78-5	-	-	-	2	1.3%	<0.1
Ferric chloride	7705-08-0	2	3	-	-	0.5%	30
Glutaraldehyde	111-30-8	1	2	2	2	23.1%	75
Glyoxal	107-22-2	>3	>3	0	2	23.0%	3.6
Hydrochloric acid	7647-01-0	1	-	2	-	54.8%	1,311
Hydrotreated light petroleum distillate	64742-47-8	-	3	2	1	32.9%	17
Isopropylbenzene	98-82-8	3	2	2	2	29.5%	0.3
Lecithins	8002-43-5	-	-	-	1	0.3%	1.4
Lithium hypochlorite	13840-33-0	1	-	1	-	0.2%	129
Naphtha (petroleum), heavy catalytic reformed	64741-68-0	-	-	-	2	0.2%	18
Naphthalene	91-20-3	1	1	1	2	48.4%	0.3
Octamethylcyclotetrasiloxane	556-67-2	-	-	-	1	0.3%	<0.1
Petroleum distillate-mineral oil grade	8002-05-9	1	-	-	1	0.1%	30
Petroleum distillates	64741-44-2	-	-	-	1	0.1%	138,679
Petroleum distillates	64742-46-7	-	-	-	1	0.1%	138,679
Poly(oxy-1,2-ethandiyl), a-(nonylphenyl)-w-hydroxy-	9016-45-9	2	-	2	2	13.2%	4.6
Polyethylene glycol monostearate	9004-99-3	-	-	-	1	1.3%	<0.1
Polypropylene	9003-07-0	-	-	-	1	1.1%	56
Polysiloxanes, di-Me	63148-62-9	3	-	-	1	1.6%	<0.1
Propargyl alcohol	107-19-7	-	2	-	>3	53.8%	3.7
Quinoline	91-22-5	3	1	-	3	18.8%	0.1
Sodium chloroacetate	3926-62-3	>3	-	-	1	0.3%	<0.1
Sodium hypochlorite	7681-52-9	1	1	1	>3	0.2%	2.3
Sodium silicate	1344-09-8	1	-	-	-	0.7%	72
Solvent naphtha, petroleum, heavy arom.	64742-94-5	1	3	2	2	39.0%	1.8
Solvent naphtha, petroleum, light arom.	64742-95-6	2	-	2	2	5.8%	1.7
Sorbitan monostearate	1338-41-6	-	-	-	1	1.3%	<0.1
Stearic acid	57-11-4	-	-	-	1	12.1%	150
Sulfonic acids, c14-16-alkane hydroxy and c14-16-alkene, sodium salts	68439-57-6	2	-	-	3	0.1%	5.4
Tall oil	8002-26-4	-	-	-	1	0.8%	13
Xylenes	1330-20-7	-	3	2	2	32.0%	1.5
Zinc sulfate	7733-02-0	1	1	1	-	0.2%	50

[a]Only chemicals with valid CASRN could be evaluated.

[b]Daphnia magna

[c]Pimephales promelas

[d]Oncorhynchus mykiss

[e]computational estimates from EPI Suite.

https://doi.org/10.1371/journal.pone.0175344.t004