

Supporting Information

An Integrative Method for Identification and Prioritization of Constituents of Concern in Produced Water from Onshore Oil and Gas Extraction

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The same documents are provided as an Excel file in electronic form

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The same documents are provided as an Excel file in electronic form.

SI Table 1. Search Logic

Database	Search Logic
PubMed	<p>(brine[Title/Abstract] OR flowback[Title/Abstract] OR wastewater[Title/Abstract] OR "produced water"[Title/Abstract] OR "produced waters"[Title/Abstract] OR "formation water"[Title/Abstract]) AND (fracking[Title/Abstract] OR frac[Title/Abstract] OR frack[Title/Abstract] OR "hydraulic fracturing"[Title/Abstract] OR unconventional[Title/Abstract] OR oilfield[Title/Abstract] OR oil-field[Title/Abstract] OR "oil field"[Title/Abstract] OR "natural gas"[Title/Abstract] OR petroleum[Title/Abstract] OR shale[Title/Abstract] OR "tight gas"[Title/Abstract] OR "tight oil"[Title/Abstract] OR conventional[Title/Abstract] OR "coalbed methane"[Title/Abstract] OR "coal-bed methane"[Title/Abstract] OR "coal bed methane"[Title/Abstract] OR CBM[Title/Abstract] OR coal seam[Title/Abstract])</p>
Web of Science	<p>TOPIC: (fracking OR frac OR frack OR "hydraulic fracturing" OR unconventional OR oil-field OR "oil field" OR oilfield OR "natural gas" OR petroleum OR shale OR "tight gas" OR "tight oil" OR conventional OR "coalbed methane" OR "coal-bed methane" OR "coal bed methane" OR CBM OR coal seam) AND TOPIC: (brine OR flowback OR wastewater OR "produced water" OR "produced waters" OR "formation water")</p>

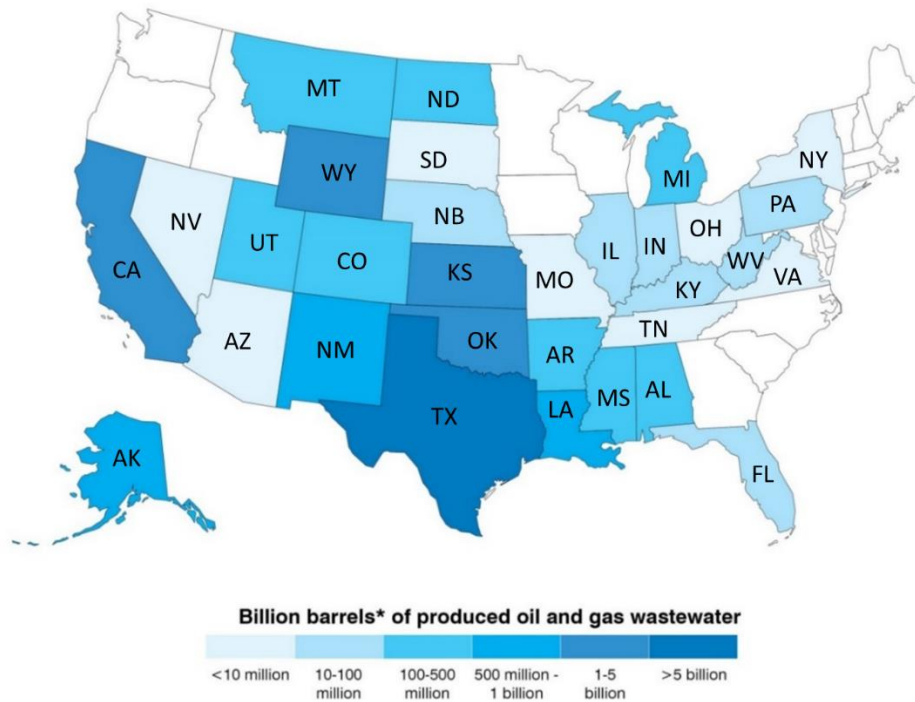
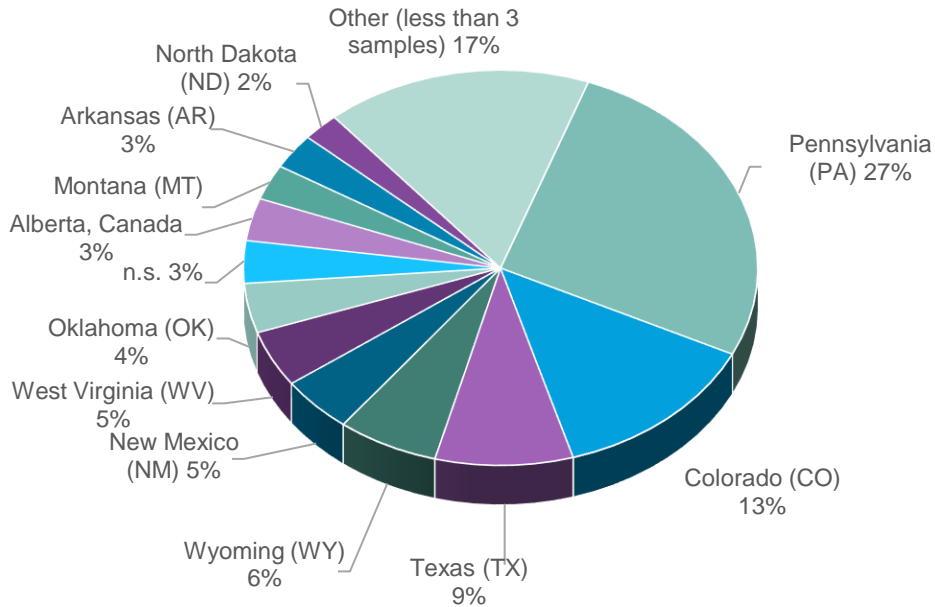
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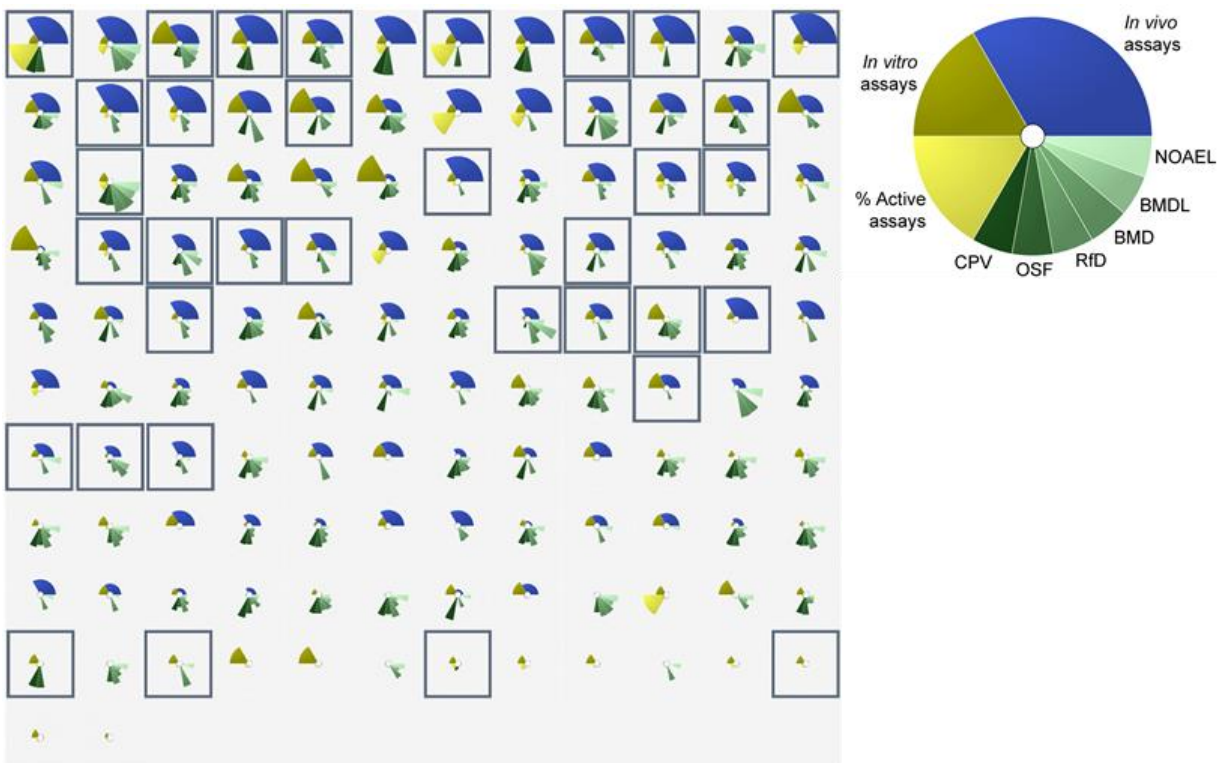
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SI Table 3: Scaling equations by domain and component.

Component (Range)	Unit	Domain	Scaling Equation
EC50 (3.7x10 ⁻⁴ to 1.2x10 ⁴)	mg/L	Ecotoxicity	$-\log_{10}[\text{EC50}] + \log_{10}(\max[\text{EC50}])$
AC50 (3.8x10 ⁻⁵ to 2.5x10 ²)	μM	Bioactivity	$-\log_{10}[\text{AC50}] + \log_{10}(\max[\text{AC50}])$
% active (0 to 41%)	%	Bioactivity	NA (Linear)
CPV (2.3 x10 ⁻³ to 21)	log ₁₀ kg·d/mol	CTV	$\log_{10}[\text{CPV}] - \log_{10}(\min[\text{CPV}])$
OSF (1.9 x10 ⁻³ to 21)	log ₁₀ kg·d/mol	CTV	$\log_{10}[\text{OSF}] - \log_{10}(\min[\text{OSF}])$
RfD (5.8 x10 ⁻⁴ to 20)	-log ₁₀ mol/(kg·d)	CTV	$-\log_{10}[\text{RfD}] + \log_{10}(\max[\text{RfD}])$
BMD (1.0 to 4.4 x10 ³)	-log ₁₀ mol/(kg·d)	CTV	$-\log_{10}[\text{BMD}] + \log_{10}(\max[\text{BMD}])$
BMDL (0.19 to 4.8 x10 ²)	-log ₁₀ mol/(kg·d)	CTV	$-\log_{10}[\text{BMDL}] + \log_{10}(\max[\text{BMDL}])$
NOAEL (0.29 to 1.0 x10 ³)	-log ₁₀ mol/(kg·d)	CTV	$-\log_{10}[\text{NOAEL}] + \log_{10}(\max[\text{NOAEL}])$



SI Figure 1. A. Distribution of samples by state. Other states/countries that represent less than 2% of total sample locations (State abbreviation, number of samples) are: Louisiana (LA, 3), Tabasco, Mexico (3), Utah (UT, 3), Alabama (AL, 3), California (CA, 2), Kansas (KS, 2), Kentucky (KY, 2), Mississippi (MS, 2), New York (NY, 2), Ohio (OH, 2), Alaska (AK, 1), British Columbia, Canada (1), Illinois (IL, 1), Indiana (IN, 1), and Nevada (NV, 1). B: Produced water intensity map developed using data from Veil 2015. *1 barrel = 42 gallons.



SI Figure 2. The sorted ToxPi profiles for all 122 the chemicals (highest in upper left moving to lowest at the bottom right). The the EPA's Priority Pollutant List (PPL) chemicals are denoted by a box (36 total compounds). ToxPi definitions are shown on the right. Each domain is represented by slices of a similar color: in vivo ecotoxicology endpoints (blue), in vitro high throughput screening assays (yellow), and known or conditional human health toxicity values (green). Individual slices represent data from related assays, endpoints, or analyses. The distance of each slice from the center indicates the normalized value of the component. The angle of the slice represents how that component is weighted relative to the other components in the overall ToxPi calculation. Cancer potency value (CPV), Oral slope factor (OSF), Reference dose (RfD), Rfd Benchmark dose (BMD), Rfd Benchmark dose lower limit (BMDL), Rfd No observed adverse effect level (NOAEL).

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
1	7440-09-7	Potassium	490	mg/L
1	14808-79-8	Sulfate	800	mg/L
1	16887-00-6	Chloride	138000	mg/L
1	18496-25-8	Sulfide	21	mg/L
1	71-52-3	Bicarbonate	167	mg/L
1	7439-95-4	Magnesium	2460	mg/L
1	7440-23-5	Sodium	69300	mg/L
1	7440-70-2	Calcium	13100	mg/L
1	7631-86-9	Silica	20	mg/L
2	7440-09-7	Potassium		
2	108-88-3	Toluene		
2	113-21-3	Lactate ion(1-)		
2	127-18-4	Tetrachloroethylene		
2	14127-61-8	Calcium ion		
2	16887-00-6	Chloride		
2	17341-25-2	Sodium ion		
2	24959-67-9	Bromide		
2	57-60-3	Pyruvate		
2	71-43-2	Benzene		
2	71-47-6	Formic acid, ion(1-)		
2	71-50-1	Acetate		
2	72-03-7	Propanoate		
2	7439-89-6	Iron		
2	7439-93-2	Lithium		
2	7439-95-4	Magnesium		
2	7439-96-5	Manganese		
2	7440-24-6	Strontium		
2	7440-39-3	Barium		
2	7440-42-8	Boron		
3	14127-61-8	Calcium ion	16509.14	mg/L
3	16887-00-6	Chloride	115277.6	mg/L
3	17341-25-2	Sodium ion	47107.2	mg/L
3	7439-89-6	Iron	19	mg/L
3	7439-95-4	Magnesium	1820.2	mg/L
3	7440-24-6	Strontium	1888.39	mg/L
3	7440-39-3	Barium	328.26	mg/L
4	12587-46-1	Alpha particle	9551	pCi/L
4	12587-47-2	Beta particle	597600	pCi/L
4	13982-63-3	Radium-226	9280	pCi/L
4	14127-61-8	Calcium ion	41000	mg/L
4	14808-79-8	Sulfate	763	mg/L
4	15117-96-1	Uranium-235	20	pCi/L
4	15262-20-1	Radium-228	1360	pCi/L
4	16887-00-6	Chloride	196000	mg/L
4	17341-25-2	Sodium ion	117000	mg/L
4	24959-67-9	Bromide	1990	mg/L
4	7439-89-6	Iron	321	mg/L
4	7439-95-4	Magnesium	2550	mg/L
4	7440-24-6	Strontium	8460	mg/L
4	7440-39-3	Barium	13800	mg/L
4	7440-61-1	Uranium	497	pCi/L
5	7440-09-7	Potassium	704	mg/L
5	14808-79-8	Sulfate	3750	mg/L
5	16887-00-6	Chloride	25690	mg/L
5	24959-67-9	Bromide	57.6	mg/L
5	71-52-3	Bicarbonate	351	mg/L
5	7439-95-4	Magnesium	525	mg/L
5	7440-23-5	Sodium	18380	mg/L
5	7440-24-6	Strontium	38	mg/L
5	7440-70-2	Calcium	1374	mg/L
6	2765-11-9	Pentadecanal	0.0453	mg/L
6	7440-09-7	Potassium	52.7	mg/L
6	10486-19-8	Tridecanal	0.0563	mg/L
6	112-54-9	Dodecanal	0.0288	mg/L
6	112-88-9	1-Octadecene	0.0463	mg/L
6	124-25-4	Tetradecanal	0.0618	mg/L
6	129-00-0	Pyrene	0.00049	mg/L
6	14797-55-8	Nitrate	171	mg/L
6	14808-79-8	Sulfate	258	mg/L
6	16887-00-6	Chloride	19912	mg/L
6	16984-48-8	Fluoride	22.8	mg/L
6	191-24-2	Benzo(g,h,i)perylene	0.00077	mg/L
6	1921-70-6	Norphytane	0.0952	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
6	193-39-5	Indeno(1,2,3-cd)pyrene	0.00076	mg/L
6	205-99-2	Benzo(b)fluoranthene	0.001	mg/L
6	207-08-9	Benzo(k)fluoranthene	0.00107	mg/L
6	218-01-9	Chrysene	0.00126	mg/L
6	50-32-8	Benzo(a)pyrene	0.00106	mg/L
6	53-70-3	Dibenz(a,h)anthracene	0.00067	mg/L
6	56-55-3	Benz(a)anthracene	0.00082	mg/L
6	629-80-1	Hexadecanal	0.165	mg/L
6	638-36-8	2,6,10,14-Tetramethylhexadecane	0.0896	mg/L
6	638-66-4	Octadecanal	0.094	mg/L
6	7373-13-9	2-Octadecanone	0.215	mg/L
6	7439-89-6	Iron	72.2	mg/L
6	7439-93-2	Lithium	10.6	mg/L
6	7439-95-4	Magnesium	79.9	mg/L
6	7439-96-5	Manganese	1.32	mg/L
6	7440-21-3	Silicon	58.7	mg/L
6	7440-23-5	Sodium	11064	mg/L
6	7440-24-6	Strontium	102	mg/L
6	7440-39-3	Barium	19.3	mg/L
6	7440-42-8	Boron	32.9	mg/L
6	7440-70-2	Calcium	682	mg/L
6	7704-34-9	Sulfur	15.7	mg/L
6	7726-95-6	Bromine	259	mg/L
6	85-01-8	Phenanthrene	0.00261	mg/L
6	86-73-7	Fluorene	0.00213	mg/L
6	91-20-3	Naphthalene	0.0247	mg/L
7	7440-09-7	Potassium	110	mg/L
7	14797-55-8	Nitrate	10	mg/L
7	14808-79-8	Sulfate	2000	mg/L
7	16887-00-6	Chloride	89690	mg/L
7	18496-25-8	Sulfide	26	mg/L
7	24959-67-9	Bromide	0.02	mg/L
7	71-52-3	Bicarbonate	152	mg/L
7	7439-89-6	Iron	30	mg/L
7	7439-95-4	Magnesium	1930	mg/L
7	7439-96-5	Manganese	0.9	mg/L
7	7440-02-0	Nickel	0.12	mg/L
7	7440-23-5	Sodium	45315	mg/L
7	7440-50-8	Copper	0.03	mg/L
7	7440-66-6	Zinc	0.04	mg/L
7	7440-70-2	Calcium	8300	mg/L
7	7631-86-9	Silica	12	mg/L
8	14808-79-8	Sulfate	2430	mg/L
8	18496-25-8	Sulfide	2	mg/L
9	7440-09-7	Potassium	6	mg/L
9	7783-06-4	Hydrogen sulfide	33	mg/L
9	14797-55-8	Nitrate	0.2	mg/L
9	16887-00-6	Chloride	161	mg/L
9	16984-48-8	Fluoride	4	mg/L
9	7429-90-5	Aluminum	0.0867	mg/L
9	7439-89-6	Iron	1.11	mg/L
9	7439-95-4	Magnesium	1.1	mg/L
9	7439-96-5	Manganese	0.0223	mg/L
9	7439-98-7	Molybdenum	0.0066	mg/L
9	7440-02-0	Nickel	0.0042	mg/L
9	7440-23-5	Sodium	721	mg/L
9	7440-33-7	Tungsten	0.0072	mg/L
9	7440-42-8	Boron	0.971	mg/L
9	7440-50-8	Copper	0.0043	mg/L
9	7440-66-6	Zinc	0.0211	mg/L
9	7440-70-2	Calcium	13.6	mg/L
10	7440-09-7	Potassium	3166	mg/L
10	14808-79-8	Sulfate	131	mg/L
10	16887-00-6	Chloride	142000	mg/L
10	24959-67-9	Bromide	860	mg/L
10	7439-89-6	Iron	20.5	mg/L
10	7439-93-2	Lithium	55.07	mg/L
10	7439-95-4	Magnesium	985.91	mg/L
10	7439-96-5	Manganese	5.99	mg/L
10	7440-17-7	Rubidium	6.251	mg/L
10	7440-21-3	Silicon	58.39	mg/L
10	7440-22-4	Silver	0.474	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
10	7440-23-5	Sodium	63110	mg/L
10	7440-24-6	Strontium	1326.6	mg/L
10	7440-28-0	Thallium	0.198	mg/L
10	7440-33-7	Tungsten	0.096	mg/L
10	7440-36-0	Antimony	0.144	mg/L
10	7440-38-2	Arsenic	0.069	mg/L
10	7440-39-3	Barium	30.95	mg/L
10	7440-42-8	Boron	298.49	mg/L
10	7440-46-2	Cesium	1.719	mg/L
10	7440-48-4	Cobalt	0.041	mg/L
10	7440-56-4	Germanium	0.161	mg/L
10	7440-65-5	Yttrium	0.011	mg/L
10	7440-69-9	Bismuth	0.424	mg/L
10	7440-70-2	Calcium	15380	mg/L
10	7553-56-2	Iodine	25.43	mg/L
10	7782-49-2	Selenium	2.241	mg/L
11	7440-09-7	Potassium	10200	mg/L
11	14808-79-8	Sulfate	694	mg/L
11	16887-00-6	Chloride	248000	mg/L
11	24959-67-9	Bromide	3670	mg/L
11	71-52-3	Bicarbonate	1370	mg/L
11	7439-89-6	Iron	393	mg/L
11	7439-93-2	Lithium	205	mg/L
11	7439-95-4	Magnesium	3810	mg/L
11	7439-96-5	Manganese	331	mg/L
11	7440-17-7	Rubidium	22.3	mg/L
11	7440-21-3	Silicon	78	mg/L
11	7440-23-5	Sodium	62400	mg/L
11	7440-24-6	Strontium	2750	mg/L
11	7440-39-3	Barium	251	mg/L
11	7440-42-8	Boron	187	mg/L
11	7440-70-2	Calcium	55700	mg/L
11	7553-56-2	Iodine	35.5	mg/L
12	7440-09-7	Potassium	11100	mg/L
12	13494-80-9	Tellurium	0.429	mg/L
12	14808-79-8	Sulfate	259	mg/L
12	16887-00-6	Chloride	180000	mg/L
12	16984-48-8	Fluoride	16.2	mg/L
12	24959-67-9	Bromide	2034	mg/L
12	71-52-3	Bicarbonate	1275	mg/L
12	7439-89-6	Iron	223	mg/L
12	7439-93-2	Lithium	51.7	mg/L
12	7439-95-4	Magnesium	1830	mg/L
12	7439-96-5	Manganese	29.6	mg/L
12	7440-17-7	Rubidium	13.5	mg/L
12	7440-21-3	Silicon	88.1	mg/L
12	7440-23-5	Sodium	82000	mg/L
12	7440-24-6	Strontium	2069	mg/L
12	7440-28-0	Thallium	0.505	mg/L
12	7440-38-2	Arsenic	0.548	mg/L
12	7440-39-3	Barium	177	mg/L
12	7440-42-8	Boron	397	mg/L
12	7440-46-2	Cesium	3.69	mg/L
12	7440-56-4	Germanium	0.44	mg/L
12	7440-70-2	Calcium	23000	mg/L
12	7553-56-2	Iodine	43.4	mg/L
12	7782-49-2	Selenium	3.74	mg/L
13	7440-09-7	Potassium	1480	mg/L
13	14127-61-8	Calcium ion	17100	mg/L
13	14808-79-8	Sulfate	619	mg/L
13	15438-31-0	Fe +2 ion	3.3	mg/L
13	16887-00-6	Chloride	67800	mg/L
13	17341-25-2	Sodium ion	41700	mg/L
13	471-34-1	Carbonic acid calcium salt (1:1)	103026	mg/L
13	7439-89-6	Iron	78	mg/L
13	7439-95-4	Magnesium	13000	mg/L
13	7439-96-5	Manganese	13.3	mg/L
13	7440-24-6	Strontium	4310	mg/L
13	7440-39-3	Barium	3850	mg/L
13	7440-70-2	Calcium	98700	mg/L
14	7440-09-7	Potassium	580	mg/L
14	7783-06-4	Hydrogen sulfide	0.6	mg/L
14	13982-63-3	Radium-226	495.4954955	pCi/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

RefId	CAS	Name	Conc (Max reported)	Units
14	14798-03-9	Ammonium	224	mg/L
14	14808-79-8	Sulfate	604	mg/L
14	16887-00-6	Chloride	130000	mg/L
14	18496-25-8	Sulfide	0.2	mg/L
14	24959-67-9	Bromide	13600	mg/L
14	71-52-3	Bicarbonate	676	mg/L
14	7439-89-6	Iron	290	mg/L
14	7439-93-2	Lithium	53	mg/L
14	7439-95-4	Magnesium	1500	mg/L
14	7439-96-5	Manganese	110	mg/L
14	7440-23-5	Sodium	52900	mg/L
14	7440-24-6	Strontium	1750	mg/L
14	7440-39-3	Barium	880	mg/L
14	7440-42-8	Boron	99	mg/L
14	7440-66-6	Zinc	73	mg/L
14	7440-70-2	Calcium	25500	mg/L
14	7631-86-9	Silica	225	mg/L
15	7440-24-6	Strontium	2698	mg/L
15	7440-70-2	Calcium	35432	mg/L
16	107-21-1	Ethylene glycol	0.38	mg/L
16	108-88-3	Toluene	0.69	mg/L
16	108-91-8	Cyclohexylamine	0.034	mg/L
16	108-95-2	Phenol	2.41	mg/L
16	110-82-7	Cyclohexane	5.97	mg/L
16	1300-71-6	Dimethylphenol	1.45	mg/L
16	1319-77-3	Cresol	2.74	mg/L
16	142-62-1	Hexanoic acid	0.22	mg/L
16	65-85-0	Benzoic acid	1.03	mg/L
16	86-55-5	1-Naphthalenecarboxylic acid	0.96	mg/L
17	14127-61-8	Calcium ion	20800	mg/L
17	16887-00-6	Chloride	159000	mg/L
17	17341-25-2	Sodium ion	49400	mg/L
17	7439-89-6	Iron	123	mg/L
17	7439-95-4	Magnesium	1992	mg/L
17	7440-24-6	Strontium	5230	mg/L
17	7440-39-3	Barium	12000	mg/L
18	7440-17-7	Rubidium	1.9	mg/L
18	7440-24-6	Strontium	660	mg/L
19	7440-09-7	Potassium	3659	mg/L
19	14808-79-8	Sulfate	260	mg/L
19	16887-00-6	Chloride	52364	mg/L
19	16984-48-8	Fluoride	1.43	mg/L
19	24959-67-9	Bromide	203	mg/L
19	71-52-3	Bicarbonate	8864	mg/L
19	7439-89-6	Iron	64.4	mg/L
19	7439-93-2	Lithium	8.9	mg/L
19	7439-95-4	Magnesium	919	mg/L
19	7439-96-5	Manganese	1.72	mg/L
19	7440-21-3	Silicon	28.9	mg/L
19	7440-23-5	Sodium	32013	mg/L
19	7440-24-6	Strontium	365	mg/L
19	7440-39-3	Barium	213	mg/L
19	7440-70-2	Calcium	2956	mg/L
20	14808-79-8	Sulfate	260	mg/L
20	16887-00-6	Chloride	52364	mg/L
20	71-52-3	Bicarbonate	8864	mg/L
20	7429-91-6	Dysprosium	0.0004	mg/L
20	7439-89-6	Iron	63.1	mg/L
20	7439-91-0	Lanthanum	0.00251	mg/L
20	7439-92-1	Lead	0.0984	mg/L
20	7439-94-3	Lutetium	0.00045	mg/L
20	7439-95-4	Magnesium	918.9	mg/L
20	7439-97-6	Mercury	0.0138	mg/L
20	7439-98-7	Molybdenum	0.4484	mg/L
20	7440-00-8	Neodymium	0.00051	mg/L
20	7440-02-0	Nickel	0.0822	mg/L
20	7440-10-0	Praseodymium	0.0004	mg/L
20	7440-19-9	Samarium	0.0012	mg/L
20	7440-23-5	Sodium	32013	mg/L
20	7440-27-9	Terbium	0.0004	mg/L
20	7440-30-4	Thulium	0.0004	mg/L
20	7440-36-0	Antimony	0.00526	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
20	7440-38-2	Arsenic	0.1647	mg/L
20	7440-42-8	Boron	30.6	mg/L
20	7440-43-9	Cadmium	0.07674	mg/L
20	7440-45-1	Cerium	0.00041	mg/L
20	7440-47-3	Chromium	0.1487	mg/L
20	7440-48-4	Cobalt	0.00978	mg/L
20	7440-50-8	Copper	1.4475	mg/L
20	7440-52-0	Erbium	0.0004	mg/L
20	7440-53-1	Europium	0.01317	mg/L
20	7440-54-2	Gadolinium	0.00277	mg/L
20	7440-60-0	Holmium	0.0004	mg/L
20	7440-62-2	Vanadium	0.2901	mg/L
20	7440-64-4	Ytterbium	0.00278	mg/L
20	7440-65-5	Yttrium	0.00279	mg/L
20	7440-66-6	Zinc	5.6385	mg/L
20	7440-70-2	Calcium	2956	mg/L
20	7782-49-2	Selenium	1.2704	mg/L
21	7440-09-7	Potassium	66000	mg/L
21	100-41-4	Ethylbenzene	1.2	mg/L
21	108-88-3	Toluene	11	mg/L
21	120-12-7	Anthracene	0.029	mg/L
21	129-00-0	Pyrene	0.23	mg/L
21	1330-20-7	Xylenes	7.6	mg/L
21	14797-55-8	Nitrate	510	mg/L
21	14808-79-8	Sulfate	5400	mg/L
21	16887-00-6	Chloride	380000	mg/L
21	16984-48-8	Fluoride	100	mg/L
21	17341-25-2	Sodium ion	130000	mg/L
21	179601-23-1	m,p-Xylene	5.5	mg/L
21	18540-29-9	Chromium (VI) ion	0.064	mg/L
21	191-24-2	Benzo(g,h,i)perylene	0.0015	mg/L
21	193-39-5	Indeno(1,2,3-cd)pyrene	0.022	mg/L
21	205-99-2	Benzo(b)fluoranthene	0.006	mg/L
21	206-44-0	Fluoranthene	0.035	mg/L
21	207-08-9	Benzo(k)fluoranthene	0.0049	mg/L
21	208-96-8	Acenaphthylene	0.11	mg/L
21	218-01-9	Chrysene	0.11	mg/L
21	24959-67-9	Bromide	360	mg/L
21	50-32-8	Benzo(a)pyrene	0.035	mg/L
21	53-70-3	Dibenz(a,h)anthracene	0.023	mg/L
21	56-55-3	Benz(a)anthracene	0.017	mg/L
21	71-43-2	Benzene	7.7	mg/L
21	7439-92-1	Lead	5.8	mg/L
21	7439-93-2	Lithium	590	mg/L
21	7439-95-4	Magnesium	9500	mg/L
21	7439-97-6	Mercury	0.011	mg/L
21	7439-98-7	Molybdenum	11	mg/L
21	7440-02-0	Nickel	1.5	mg/L
21	7440-22-4	Silver	2	mg/L
21	7440-24-6	Strontium	3400	mg/L
21	7440-28-0	Thallium	10	mg/L
21	7440-36-0	Antimony	12	mg/L
21	7440-38-2	Arsenic	15	mg/L
21	7440-39-3	Barium	160000	mg/L
21	7440-41-7	Beryllium	0.29	mg/L
21	7440-42-8	Boron	420	mg/L
21	7440-43-9	Cadmium	0.6	mg/L
21	7440-47-3	Chromium	0.16	mg/L
21	7440-48-4	Cobalt	1.2	mg/L
21	7440-50-8	Copper	7.9	mg/L
21	7440-61-1	Uranium	95	pCi/L
21	7440-62-2	Vanadium	0.73	mg/L
21	7440-66-6	Zinc	9.4	mg/L
21	7440-70-2	Calcium	180000	mg/L
21	74-82-8	Methane	15	mg/L
21	7782-49-2	Selenium	17	mg/L
21	83-32-9	Acenaphthene	0.28	mg/L
21	85-01-8	Phenanthrene	1.2	mg/L
21	86-73-7	Fluorene	0.51	mg/L
21	91-20-3	Naphthalene	2.3	mg/L
21	95-47-6	o-Xylene	2.1	mg/L
22	14265-44-2	Phosphate	1.1	mg/L
22	14808-79-8	Sulfate	67	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
22	16887-00-6	Chloride	20406	mg/L
22	7439-89-6	Iron	0.3	mg/L
22	7439-95-4	Magnesium	459	mg/L
22	7440-23-5	Sodium	8997	mg/L
22	7440-39-3	Barium	8.5	mg/L
22	7440-42-8	Boron	132	mg/L
22	7440-70-2	Calcium	1095	mg/L
22	7631-86-9	Silica	181	mg/L
22	7664-41-7	Ammonia	0.4	mg/L
23	7440-09-7	Potassium	516	mg/L
23	108-88-3	Toluene		
23	1120-21-4	Undecane		
23	112-40-3	Dodecane		
23	119-64-2	Tetralin		
23	1321-94-4	Methylnaphthalene		
23	1330-20-7	Xylenes		
23	14127-61-8	Calcium ion	8340	mg/L
23	15438-31-0	Fe +2 ion	126	mg/L
23	16887-00-6	Chloride	95100	mg/L
23	17341-25-2	Sodium ion	30500	mg/L
23	24959-67-9	Bromide	939	mg/L
23	25551-13-7	Trimethylbenzene		
23	64-19-7	Acetic acid		
23	71-43-2	Benzene		
23	7439-95-4	Magnesium	1188	mg/L
23	7440-39-3	Barium	3386	mg/L
23	7704-34-9	Sulfur	11.7	mg/L
23	7723-14-0	Phosphorus	8.8	mg/L
23	91-20-3	Naphthalene		
24	7440-09-7	Potassium	970	mg/L
24	7783-06-4	Hydrogen sulfide	190	mg/L
24	100-41-4	Ethylbenzene	0.024	mg/L
24	108-88-3	Toluene	0.078	mg/L
24	12587-46-1	Alpha particle	46.1	pCi/L
24	12587-47-2	Beta particle	122	pCi/L
24	1330-20-7	Xylenes	0.327	mg/L
24	14265-44-2	Phosphate	9.42	mg/L
24	14808-79-8	Sulfate	1800	mg/L
24	14859-67-7	Radon 222	139	pCi/L
24	16887-00-6	Chloride	20100	mg/L
24	16984-48-8	Fluoride	20	mg/L
24	24959-67-9	Bromide	69.6	mg/L
24	3812-32-6	Carbonate	1178	mg/L
24	471-34-1	Carbonic acid calcium salt (1:1)	11400	mg/L
24	57-12-5	Cyanide	3	mg/L
24	71-43-2	Benzene	0.5	mg/L
24	71-52-3	Bicarbonate	13900	mg/L
24	7429-90-5	Aluminum	2.9	mg/L
24	7439-89-6	Iron	258	mg/L
24	7439-92-1	Lead	0.39	mg/L
24	7439-93-2	Lithium	4.73	mg/L
24	7439-95-4	Magnesium	511	mg/L
24	7439-96-5	Manganese	2	mg/L
24	7439-98-7	Molybdenum	0.049	mg/L
24	7440-02-0	Nickel	2.61	mg/L
24	7440-22-4	Silver	0.14	mg/L
24	7440-23-5	Sodium	7834	mg/L
24	7440-24-6	Strontium	47.9	mg/L
24	7440-31-5	Tin	0.039	mg/L
24	7440-32-6	Titanium	0.02	mg/L
24	7440-38-2	Arsenic	0.3	mg/L
24	7440-39-3	Barium	74	mg/L
24	7440-42-8	Boron	4.7	mg/L
24	7440-43-9	Cadmium	0.006	mg/L
24	7440-47-3	Chromium	3.71	mg/L
24	7440-48-4	Cobalt	0.018	mg/L
24	7440-50-8	Copper	4.6	mg/L
24	7440-61-1	Uranium	2.5	mg/L
24	7440-62-2	Vanadium	0.013	mg/L
24	7440-66-6	Zinc	3.9	mg/L
24	7440-70-2	Calcium	5530	mg/L
24	7631-86-9	Silica	37.75	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
24	7727-37-9	Nitrogen	26.1	mg/L
24	7782-49-2	Selenium	0.119	mg/L
25	7429-90-5	Aluminum	0.11	mg/L
25	7439-89-6	Iron	8.3	mg/L
25	7439-95-4	Magnesium	16.2	mg/L
25	7439-96-5	Manganese	0.14	mg/L
25	7440-02-0	Nickel	0.015	mg/L
25	7440-24-6	Strontium	6.5	mg/L
25	7440-39-3	Barium	12.6	mg/L
25	7440-50-8	Copper	0.06	mg/L
25	7440-66-6	Zinc	0.1	mg/L
25	7440-70-2	Calcium	40	mg/L
26	7440-09-7	Potassium	6000	mg/L
26	100-41-4	Ethylbenzene	4410	mg/L
26	103-65-1	Propylbenzene	1290	mg/L
26	104-51-8	Butylbenzene	162	mg/L
26	105-67-9	2,4-Dimethylphenol	5	mg/L
26	108-67-8	1,3,5-Trimethylbenzene	6250	mg/L
26	108-88-3	Toluene	16800	mg/L
26	108-95-2	Phenol	6.96	mg/L
26	112-27-6	Triethylene glycol	17.8	mg/L
26	1319-77-3	Cresol	6.76	mg/L
26	135-98-8	sec-Butylbenzene	270	mg/L
26	14127-61-8	Calcium ion	1771	mg/L
26	14808-79-8	Sulfate	2100	mg/L
26	15438-31-0	Fe +2 ion	190.6	mg/L
26	16887-00-6	Chloride	5945	mg/L
26	179601-23-1	m,p-Xylene	46000	mg/L
26	281-23-2	Adamantane	74	mg/L
26	3812-32-6	Carbonate	17000	mg/L
26	702-79-4	1,3-Dimethyladamantane	9.8	mg/L
26	71-43-2	Benzene	860	mg/L
26	71-52-3	Bicarbonate	4301	mg/L
26	7439-95-4	Magnesium	131	mg/L
26	7440-23-5	Sodium	2700	mg/L
26	75-09-2	Dichloromethane	0.51	mg/L
26	91-20-3	Naphthalene	37.8	mg/L
26	91-57-6	2-Methylnaphthalene	110	mg/L
26	95-47-6	o-Xylene	9430	mg/L
26	95-48-7	o-Cresol	7.76	mg/L
26	95-63-6	1,2,4-Trimethylbenzene	8730	mg/L
26	98-06-6	tert-Butylbenzene	86	mg/L
26	98-82-8	Cumene	948	mg/L
26	99-87-6	p-Cymene	334	mg/L
27	13982-63-3	Radium-226		
28	7440-09-7	Potassium	1410	mg/L
28	14808-79-8	Sulfate	1790	mg/L
28	15438-31-0	Fe +2 ion	206.7790968	mg/L
28	16887-00-6	Chloride	97600	mg/L
28	17341-25-2	Sodium ion	54600	mg/L
28	18496-25-8	Sulfide	33.9	mg/L
28	24959-67-9	Bromide	1220	mg/L
28	7439-95-4	Magnesium	1310	mg/L
28	7439-96-5	Manganese	8.549077085	mg/L
28	7440-21-3	Silicon	30.53462607	mg/L
28	7440-24-6	Strontium	1900	mg/L
28	7440-39-3	Barium	411.1584049	mg/L
28	7440-42-8	Boron	50.3	mg/L
28	7440-70-2	Calcium	8010	mg/L
28	7553-56-2	Iodine	385	mg/L
28	7664-41-7	Ammonia	1970	mg/L
29	16887-00-6	Chloride	22209	mg/L
29	7429-90-5	Aluminum	1.6	mg/L
29	7439-89-6	Iron	189	mg/L
29	7439-95-4	Magnesium	54.8	mg/L
29	7440-24-6	Strontium	52.7	mg/L
29	7440-39-3	Barium	30.6	mg/L
29	7440-42-8	Boron	23.5	mg/L
29	7440-70-2	Calcium	397	mg/L
30	7440-09-7	Potassium	51.6	mg/L
30	14808-79-8	Sulfate	4.2	mg/L
30	16887-00-6	Chloride	15550	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
30	17341-25-2	Sodium ion	9372	mg/L
30	24959-67-9	Bromide	68	mg/L
30	71-52-3	Bicarbonate	840	mg/L
30	7429-90-5	Aluminum	1.3	mg/L
30	7439-89-6	Iron	65.4	mg/L
30	7439-95-4	Magnesium	68.2	mg/L
30	7439-96-5	Manganese	0.8	mg/L
30	7440-21-3	Silicon	63.5	mg/L
30	7440-24-6	Strontium	53.1	mg/L
30	7440-41-7	Beryllium	18.2	mg/L
30	7440-42-8	Boron	18.5	mg/L
30	7440-50-8	Copper	0.1	mg/L
30	7440-70-2	Calcium	453	mg/L
30	7664-41-7	Ammonia	40	mg/L
31	7440-09-7	Potassium	37.1	mg/L
31	16887-00-6	Chloride	7082	mg/L
31	16984-48-8	Fluoride	15.22	mg/L
31	24959-67-9	Bromide	55	mg/L
31	3812-32-6	Carbonate	217.7	mg/L
31	71-52-3	Bicarbonate	6417	mg/L
31	7439-89-6	Iron	10	mg/L
31	7439-93-2	Lithium	1.18	mg/L
31	7439-95-4	Magnesium	45.6	mg/L
31	7439-96-5	Manganese	0.33	mg/L
31	7440-23-5	Sodium	4160	mg/L
31	7440-39-3	Barium	15.1	mg/L
31	7440-50-8	Copper	0.059	mg/L
31	7440-70-2	Calcium	163.6	mg/L
32	111-30-8	Glutaraldehyde		
32	63449-41-2	Benzyl-C8-18-alkyldimethylammonium chlorides		
32	68139-30-0	1-Propanaminium, N-(3-aminopropyl)-2-hydroxy-N,N-dimethyl-3-sulfo-, N-coco acyl derivs., inner salts		
32	68140-01-2	N-[3-(Dimethylamino)propyl] coco amides		
32	9000-30-0	Guar gum		
33	7440-42-8	Boron	310	mg/L
34	7440-09-7	Potassium	140	mg/L
34	100-41-4	Ethylbenzene	0.0089	mg/L
34	105-67-9	2,4-Dimethylphenol	0.0066	mg/L
34	106-44-5	p-Cresol	0.031	mg/L
34	108-88-3	Toluene	0.11	mg/L
34	108-95-2	Phenol	0.009	mg/L
34	129-00-0	Pyrene	0.0019	mg/L
34	132-64-9	Dibenzofuran	0.0036	mg/L
34	1330-20-7	Xylenes	0.13	mg/L
34	14808-79-8	Sulfate	2500	mg/L
34	16887-00-6	Chloride	1500	mg/L
34	16984-48-8	Fluoride	4.4	mg/L
34	208-96-8	Acenaphthylene	0.0021	mg/L
34	471-34-1	Carbonic acid calcium salt (1:1)	3540	mg/L
34	67-64-1	Acetone	0.62	mg/L
34	71-43-2	Benzene	0.04	mg/L
34	7439-95-4	Magnesium	54	mg/L
34	7440-23-5	Sodium	970	mg/L
34	7440-70-2	Calcium	370	mg/L
34	7727-37-9	Nitrogen	0.06	mg/L
34	78-93-3	Methyl ethyl ketone	0.0015	mg/L
34	83-32-9	Acenaphthene	0.0033	mg/L
34	85-01-8	Phenanthrene	0.01	mg/L
34	86-73-7	Fluorene	0.002	mg/L
34	91-20-3	Naphthalene	0.021	mg/L
34	91-57-6	2-Methylnaphthalene	0.1	mg/L
34	95-48-7	o-Cresol	0.0078	mg/L
35	10023-74-2	Pentanoic acid, ion(1-)	1.51689	mg/L
35	103-40-2	Benzylsuccinate	0.006871029	mg/L
35	106-65-0	Dimethyl succinate	0.8914662	mg/L
35	108-95-2	Phenol	0.7999605	mg/L
35	110-94-1	Glutaric acid	0.290653	mg/L
35	111-14-8	Heptanoic acid	0.3124488	mg/L
35	111-16-0	Heptanedioic acid	0.1441521	mg/L
35	1131-63-1	5,6,7,8-Tetrahydro-2-naphthoic acid	0.002995655	mg/L
35	118-90-1	2-Methylbenzoic acid	0.21784	mg/L
35	121-91-5	1,3-Benzenedicarboxylic acid	0.3821036	mg/L
35	123-25-1	Diethyl butanedioate	1.4109876	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
35	124-07-2	Octanoic acid	0.08220198	mg/L
35	142-62-1	Hexanoic acid	0.766656	mg/L
35	533-18-6	Acetic acid, 2-methylphenyl ester	0.05556549	mg/L
35	766-76-7	Benzoate	0.3512364	mg/L
35	86-55-5	1-Naphthalenecarboxylic acid	0.003615843	mg/L
35	93-09-4	2-Naphthalenecarboxylic acid	0.02582745	mg/L
35	95-48-7	o-Cresol	0.248722	mg/L
35	99-06-9	3-Hydroxybenzoic acid	0.03038684	mg/L
36	7440-09-7	Potassium		
36	7439-89-6	Iron		
36	7439-95-4	Magnesium		
36	7440-23-5	Sodium		
36	7440-24-6	Strontium		
36	7440-39-3	Barium		
36	7440-70-2	Calcium		
37	14798-03-9	Ammonium		
37	16887-00-6	Chloride		
37	24959-67-9	Bromide		
37	7553-56-2	Iodine		
38	7440-09-7	Potassium		
38	100-41-4	Ethylbenzene		
38	100-51-6	Benzyl alcohol		
38	1024-57-3	Heptachlor epoxide		
38	103-65-1	Propylbenzene		
38	104-51-8	Butylbenzene		
38	105-67-9	2,4-Dimethylphenol		
38	10595-95-6	N-Nitroso-N-methylethylamine		
38	106-44-5	p-Cresol		
38	107-02-8	Acrolein		
38	107-13-1	Acrylonitrile		
38	107-21-1	Ethylene glycol		
38	107-92-6	Butanoic acid		
38	108-39-4	m-Cresol		
38	108-67-8	1,3,5-Trimethylbenzene		
38	108-88-3	Toluene		
38	108-95-2	Phenol		
38	109-06-8	2-Methylpyridine		
38	110-86-1	Pyridine		
38	111-44-4	Bis(2-chloroethyl) ether		
38	117-81-7	Di(2-ethylhexyl) phthalate		
38	117-84-0	Di-n-octyl phthalate		
38	120-82-1	1,2,4-Trichlorobenzene		
38	122-39-4	Diphenylamine		
38	123-91-1	1,4-Dioxane		
38	124-38-9	Carbon dioxide		
38	12672-29-6	Aroclor 1248		
38	127-18-4	Tetrachloroethylene		
38	129-00-0	Pyrene		
38	1330-20-7	Xylenes		
38	135-98-8	sec-Butylbenzene		
38	14797-55-8	Nitrate		
38	14797-65-0	Nitrite		
38	14808-79-8	Sulfate		
38	16887-00-6	Chloride		
38	16984-48-8	Fluoride		
38	18496-25-8	Sulfide		
38	191-24-2	Benzo(g,h,i)perylene		
38	193-39-5	Indeno(1,2,3-cd)pyrene		
38	205-99-2	Benzo(b)fluoranthene		
38	206-44-0	Fluoranthene		
38	207-08-9	Benzo(k)fluoranthene		
38	24959-67-9	Bromide		
38	298-02-2	Phorate		
38	309-00-2	Aldrin		
38	319-85-7	beta-Hexachlorocyclohexane		
38	319-86-8	delta-Hexachlorocyclohexane		
38	33213-65-9	Endosulfan II		
38	50-32-8	Benzo(a)pyrene		
38	53-70-3	Dibenz(a,h)anthracene		
38	57-12-5	Cyanide		
38	57-55-6	1,2-Propylene glycol		
38	57-97-6	7,12-Dimethylbenz(a)anthracene		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
38	58-89-9	Lindane		
38	60-57-1	Dieldrin		
38	64-19-7	Acetic acid		
38	67-56-1	Methanol		
38	67-63-0	Isopropanol		
38	67-64-1	Acetone		
38	67-66-3	Chloroform		
38	71-43-2	Benzene		
38	72-55-9	p,p'-DDE		
38	7421-93-4	Endrin aldehyde		
38	7429-90-5	Aluminum		
38	7439-89-6	Iron		
38	7439-92-1	Lead		
38	7439-93-2	Lithium		
38	7439-95-4	Magnesium		
38	7439-96-5	Manganese		
38	7439-97-6	Mercury		
38	7439-98-7	Molybdenum		
38	7440-02-0	Nickel		
38	7440-22-4	Silver		
38	7440-23-5	Sodium		
38	7440-24-6	Strontium		
38	7440-28-0	Thallium		
38	7440-31-5	Tin		
38	7440-32-6	Titanium		
38	7440-36-0	Antimony		
38	7440-38-2	Arsenic		
38	7440-39-3	Barium		
38	7440-41-7	Beryllium		
38	7440-42-8	Boron		
38	7440-43-9	Cadmium		
38	7440-47-3	Chromium		
38	7440-48-4	Cobalt		
38	7440-50-8	Copper		
38	7440-66-6	Zinc		
38	7440-67-7	Zirconium		
38	7440-70-2	Calcium		
38	74-83-9	Methyl bromide		
38	75-09-2	Dichloromethane		
38	75-15-0	Carbon disulfide		
38	75-25-2	Bromoform		
38	7553-56-2	Iodine		
38	76-44-8	Heptachlor		
38	7664-41-7	Ammonia		
38	7723-14-0	Phosphorus		
38	7782-49-2	Selenium		
38	78-93-3	Methyl ethyl ketone		
38	84-66-2	Diethyl phthalate		
38	84-74-2	Dibutyl phthalate		
38	85-01-8	Phenanthrene		
38	86-30-6	N-Nitrosodiphenylamine		
38	86-73-7	Fluorene		
38	87-61-6	1,2,3-Trichlorobenzene		
38	87-65-0	2,6-Dichlorophenol		
38	91-20-3	Naphthalene		
38	91-57-6	2-Methylnaphthalene		
38	94-59-7	Safrole		
38	95-48-7	o-Cresol		
38	95-63-6	1,2,4-Trimethylbenzene		
38	959-98-8	Endosulfan I		
38	98-82-8	Cumene		
38	98-86-2	Acetophenone		
38	99-87-6	p-Cymene		
39	100-51-6	Benzyl alcohol		
39	105-67-9	2,4-Dimethylphenol		
39	10595-95-6	N-Nitroso-N-methylethylamine		
39	106-44-5	p-Cresol		
39	108-39-4	m-Cresol		
39	108-67-8	1,3,5-Trimethylbenzene		
39	108-95-2	Phenol		
39	110-86-1	Pyridine		
39	120-83-2	2,4-Dichlorophenol		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
39	122-39-4	Diphenylamine		
39	122-66-7	1,2-Diphenylhydrazine		
39	123-91-1	1,4-Dioxane		
39	129-00-0	Pyrene		
39	191-24-2	Benzo(g,h,i)perylene		
39	193-39-5	Indeno(1,2,3-cd)pyrene		
39	205-99-2	Benzo(b)fluoranthene		
39	206-44-0	Fluoranthene		
39	207-08-9	Benzo(k)fluoranthene		
39	218-01-9	Chrysene		
39	50-32-8	Benzo(a)pyrene		
39	53-70-3	Dibenz(a,h)anthracene		
39	56-55-3	Benz(a)anthracene		
39	67-64-1	Acetone		
39	85-01-8	Phenanthrene		
39	86-30-6	N-Nitrosodiphenylamine		
39	86-73-7	Fluorene		
39	91-20-3	Naphthalene		
39	91-57-6	2-Methylnaphthalene		
39	92-87-5	Benzidine		
39	95-48-7	o-Cresol		
39	95-63-6	1,2,4-Trimethylbenzene		
39	98-86-2	Acetophenone		
40	13982-63-3	Radium-226	15570	pCi/L
40	14127-61-8	Calcium ion	31270	mg/L
40	15262-20-1	Radium-228	1385	pCi/L
40	15438-31-0	Fe +2 ion	28.2	mg/L
40	16887-00-6	Chloride	152213	mg/L
40	17341-25-2	Sodium ion	31382	mg/L
40	7439-95-4	Magnesium	1590	mg/L
40	7440-24-6	Strontium	16141	mg/L
40	7440-39-3	Barium	19115	mg/L
41	7440-09-7	Potassium	2570	mg/L
41	115-86-6	Triphenyl phosphate		
41	120-12-7	Anthracene	0.0000507	mg/L
41	129-00-0	Pyrene	0.0000373	mg/L
41	132-65-0	Dibenzothiophene	0.0000237	mg/L
41	14127-61-8	Calcium ion	11800	mg/L
41	1576-67-6	3,6-Dimethylphenanthrene	0.000334	mg/L
41	16887-00-6	Chloride	136000	mg/L
41	1730-37-6	1-Methylfluorene	0.000297	mg/L
41	205-82-3	Benzo(j)fluoranthene		
41	205-99-2	Benzo(b)fluoranthene	0.0000103	mg/L
41	206-44-0	Fluoranthene	0.00000961	mg/L
41	207-08-9	Benzo(k)fluoranthene		
41	208-96-8	Acenaphthylene	0.0000137	mg/L
41	218-01-9	Chrysene	0.0000502	mg/L
41	2381-21-7	1-Methylpyrene	0.0000477	mg/L
41	25322-68-3	Polyethylene glycol		
41	483-65-8	Retene	0.0000336	mg/L
41	50-32-8	Benzo(a)pyrene	0.0000112	mg/L
41	56-55-3	Benz(a)anthracene	0.0000159	mg/L
41	7440-23-5	Sodium	70000	mg/L
41	7727-37-9	Nitrogen	498	mg/L
41	832-69-9	1-Methyl phenanthrene	0.000234	mg/L
41	83-32-9	Acenaphthene	0.000028	mg/L
41	85-01-8	Phenanthrene	0.000145	mg/L
41	86-73-7	Fluorene	0.000545	mg/L
41	90-12-0	1-Methylnaphthalene	0.000111	mg/L
41	91-20-3	Naphthalene	0.0000563	mg/L
41	95906-11-9	tris(2,4-di-tert-butylphenyl) phosphate		
42	120-12-7	Anthracene		
42	129-00-0	Pyrene		
42	1576-67-6	3,6-Dimethylphenanthrene		
42	1730-37-6	1-Methylfluorene		
42	191-24-2	Benzo(g,h,i)perylene		
42	205-99-2	Benzo(b)fluoranthene		
42	206-44-0	Fluoranthene		
42	218-01-9	Chrysene		
42	2381-21-7	1-Methylpyrene		
42	53-70-3	Dibenz(a,h)anthracene		
42	56-55-3	Benz(a)anthracene		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
42	832-69-9	1-Methyl phenanthrene		
42	85-01-8	Phenanthrene		
42	86-73-7	Fluorene		
43	7440-09-7	Potassium	48.14	mg/L
43	14265-44-2	Phosphate	8.34	mg/L
43	14808-79-8	Sulfate	2582	mg/L
43	16887-00-6	Chloride	2139	mg/L
43	16984-48-8	Fluoride	3.62	mg/L
43	24959-67-9	Bromide	0.04	mg/L
43	71-52-3	Bicarbonate	5368	mg/L
43	7429-90-5	Aluminum	105	mg/L
43	7439-89-6	Iron	162	mg/L
43	7439-92-1	Lead	0.51	mg/L
43	7439-93-2	Lithium	0.32	mg/L
43	7439-95-4	Magnesium	54.92	mg/L
43	7439-96-5	Manganese	2.69	mg/L
43	7440-02-0	Nickel	0.56	mg/L
43	7440-21-3	Silicon	51.38	mg/L
43	7440-23-5	Sodium	2539	mg/L
43	7440-24-6	Strontium	6.69	mg/L
43	7440-39-3	Barium	375	mg/L
43	7440-42-8	Boron	4.1	mg/L
43	7440-47-3	Chromium	3.16	mg/L
43	7440-50-8	Copper	0.91	mg/L
43	7440-62-2	Vanadium	0.34	mg/L
43	7440-66-6	Zinc	1.3	mg/L
43	7440-70-2	Calcium	544	mg/L
44	2883-02-5	Cyclohexane, nonyl-		
44	4810-04-2	1,3,5-Trimethyl-2-propylbenzene		
44	5161-04-6	Benzene, 1-methyl-4-(2-methylpropyl)-		
44	5911-04-6	3-Methylnonane		
44	1002-43-3	Undecane, 3-methyl-		
44	100-41-4	Ethylbenzene		
44	100-51-6	Benzyl alcohol		
44	100-52-7	Benzaldehyde		
44	1008-80-6	2,3-Dimethyldecahydronaphthalene		
44	101-81-5	Diphenylmethane		
44	10222-95-4	5-Isopropyl-1,2,4-trimethylbenzene		
44	10317-17-6	Oxetane, 3-(1-methylethyl)-		
44	103-65-1	Propylbenzene		
44	10374-74-0	7-Tetradecene		
44	104-50-7	4-Octanolide		
44	104-51-8	Butylbenzene		
44	104-61-0	gamma-Nonanolactone		
44	104-76-7	2-Ethyl-1-hexanol		
44	105-21-5	1,4-Heptanolide		
44	10522-26-6	2-Methyl-1-undecanol		
44	10544-95-3	Octadecane, 4-methyl-		
44	106-21-8	3,7-Dimethyloctan-1-ol		
44	106-35-4	3-Heptanone		
44	106-42-3	p-Xylene		
44	106-44-5	p-Cresol		
44	1075-06-5	Ethanone, 2,2-dihydroxy-1-phenyl-		
44	1077-16-3	Benzene, hexyl-		
44	107-92-6	Butanoic acid		
44	1079-71-6	1,2,3,4,5,6,7,8-Octahydroanthracene		
44	1081-77-2	1-Phenylnonane		
44	108-29-2	4-Pentanolide		
44	108-88-3	Toluene		
44	108-94-1	Cyclohexanone		
44	108-95-2	Phenol		
44	109-52-4	Pentanoic acid		
44	111-14-8	Heptanoic acid		
44	111-27-3	1-Hexanol		
44	111-65-9	Octane		
44	111-76-2	2-Butoxyethanol		
44	111-84-2	Nonane		
44	1120-21-4	Undecane		
44	112-05-0	Nonanoic acid		
44	112-30-1	1-Decanol		
44	112-31-2	Decanal		
44	112-37-8	Undecanoic acid		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
44	112-40-3	Dodecane		
44	1124-63-6	3-Cyclohexylpropan-1-ol		
44	112-70-9	1-Tridecanol		
44	1129-29-9	1-Isopropenyl-3-isopropylbenzene		
44	115-22-0	2-Butanone, 3-hydroxy-3-methyl-		
44	116-53-0	2-Methylbutanoic acid		
44	119-64-2	Tetralin		
44	123-05-7	2-Ethylhexanal		
44	123-20-6	Butanoic acid, ethenyl ester		
44	124-07-2	Octanoic acid		
44	124-10-7	Methyl tetradecanoate		
44	124-18-5	Decane		
44	13151-94-5	1,2-Dimethylcyclooctane		
44	13286-73-2	3-Ethyltridecane		
44	13287-21-3	6-Methyltridecane		
44	13287-23-5	8-Methylheptadecane		
44	13432-25-2	3-hexanol, 2,4-dimethyl-		
44	135-98-8	sec-Butylbenzene		
44	13632-94-5	1,4-Diethyl-2-methylbenzene		
44	13833-20-0	Amorphane		
44	140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol		
44	14123-41-2	3-Chloro-1,1,2,2-tetramethylcyclopropane		
44	14250-88-5	2,2-Dimethylvaleraldehyde		
44	142-62-1	Hexanoic acid		
44	14276-95-0	1H-Indene, 2,3-dihydro-1,1,6-trimethyl-		
44	143-07-7	Dodecanoic acid		
44	143-08-8	1-Nonanol		
44	14398-67-5	Decalin, syn-1-methyl-, cis-		
44	14398-71-1	cis-Decalin, 2-syn-methyl-		
44	1468-39-9	2-Methylbutanoic anhydride		
44	146919-79-1	5-Methyl-1-undecene		
44	149-57-5	2-Ethylhexanoic acid		
44	15232-85-6	Cyclohexene, 1-pentyl-		
44	15232-86-7	1-Heptylcyclohexene		
44	1559-81-5	1-Methyltetraline		
44	1560-88-9	Octadecane, 2-methyl-		
44	1560-89-0	Heptadecane, 2-methyl-		
44	1560-92-5	2-Methylhexadecane		
44	1560-93-6	2-Methylpentadecane		
44	1560-95-8	2-Methyltetradecane		
44	1560-96-9	2-Methyltridecane		
44	1560-97-0	2-Methyldodecane		
44	1595-10-4	1-Methyl-2-n-hexylbenzene		
44	1595-16-0	1-(Butan-2-yl)-4-methylbenzene		
44	1599-67-3	1-Docosene		
44	1606-08-2	Cyclopentylcyclohexane		
44	1618-22-0	naphthalene, decahydro-2,6-dimethyl-		
44	1632-70-8	Undecane, 5-methyl-		
44	16538-89-9	cyclooctane, (1-methylpropyl)-		
44	16580-24-8	1-Methyl-3-propan-2-ylcyclohexane		
44	16580-26-0	cyclohexane, 1-isopropyl-1-methyl-		
44	1660-04-4	Methyl tricyclo(3.3.1.13,7)dec-1-yl ketone		
44	1678-93-9	Butylcyclohexane		
44	1687-34-9	1-Ethyl-3-methyladamantane		
44	1687-64-5	Phenol, 2-ethyl-6-methyl-		
44	1703-51-1	2,5-Heptanedione		
44	17059-48-2	1H-Indene, 2,3-dihydro-1,6-dimethyl-		
44	17301-23-4	2,6-Dimethylundecane		
44	17301-26-7	2,9-Dimethylundecane		
44	17302-28-2	Nonane, 2,6-dimethyl-		
44	17302-32-8	3,7-Dimethylnonane		
44	17312-54-8	3,7-Dimethyldecane		
44	17312-57-1	3-Methyldodecane		
44	17312-81-1	3,5-Dimethylundecane		
44	17429-36-6	2-Cyclohexen-1-one, 4-methyl-4-phenyl-		
44	17453-94-0	Undecane, 5-ethyl-		
44	1746-23-2	4-tert-Butylstyrene		
44	1750-51-2	Naphthalene, decahydro-1,6-dimethyl-		
44	1758-88-9	2-Ethyl-p-xylene		
44	17720-63-7	N,N,O-Triacetylhydroxylamine		
44	17851-53-5	Butyl isobutyl phthalate		
44	1795-15-9	Cyclohexane, octyl-		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
44	1795-16-0	Decylcyclohexane		
44	18420-41-2	2-(Chloromethyl)tetrahydropyran		
44	18435-22-8	Tetradecane, 3-methyl-		
44	18435-45-5	1-Nonadecene		
44	1871-67-6	2-Octenoic acid		
44	1921-70-6	Norphytane		
44	19218-94-1	1-Iodotetradecane		
44	19219-84-2	benzene, (1,3-dimethylbutyl)-		
44	19781-34-1	3-ethyl-3-phenyl-1-pentene		
44	1985-59-7	1,1-Dimethyl(1,2,3,4-tetrahydronaphthalene)		
44	1985-88-2	4-Chloro-2-methyl-2-butanol		
44	1985-97-3	(3-methylpentan-3-yl)benzene		
44	2027-17-0	2-Isopropyl-naphthalene		
44	2049-95-8	tert-Pentylbenzene		
44	2082-59-9	valeric anhydride		
44	20959-33-5	Heptadecane, 7-methyl-		
44	21195-59-5	1,5,8-p-Menthatriene		
44	2131-41-1	1,4,5-Trimethylnaphthalene		
44	21524-26-5	Cyclohexene, 4-butyl-		
44	21693-54-9	5,7-Dimethyltetralin		
44	2189-60-8	Benzene, octyl-		
44	22089-89-0	7-pentadecyne		
44	2216-34-4	4-Methyloctane		
44	2234-20-0	2,4-Dimethylstyrene		
44	2245-38-7	1,6,7-Trimethylnaphthalene		
44	22531-20-0	6-Ethyl-1,2,3,4-tetrahydronaphthalene		
44	2292-79-7	Congressane		
44	23051-84-5	5-Tridecene, (5E)-		
44	23342-25-8	2,2,5,7-Tetramethyltetralin		
44	23609-46-3	cyclooctane, 1,2-diethyl-		
44	2363-88-4	2,4-Decadienal		
44	2399-48-6	Tetrahydrofurfuryl acrylate		
44	2416-20-8	hexadecenoic acid, z-11-		
44	2435-85-0	Hexadecahydropyrene		
44	25117-24-2	4-Methyltetradecane		
44	25117-31-1	5-Methyltridecane		
44	25117-32-2	5-Methyltetradecane		
44	25117-35-5	Octadecane, 5-methyl-		
44	25419-33-4	naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-		
44	25524-42-9	5-Tridecene, (Z)-		
44	26429-11-8	4-Methylheptadecane		
44	26730-12-1	4-Methyltridecane		
44	26730-20-1	7-Methylhexadecane		
44	27554-26-3	Diisooctyl phthalate		
44	28071-99-0	trans-anti-trans-tetra-decahydroanthracene		
44	2809-64-5	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-		
44	286-20-4	Cyclohexene oxide		
44	2882-96-4	pentadecane, 3-methyl-		
44	28980-74-7	3,5-Dodecadiene, 2-methyl-		
44	294-62-2	Cyclododecane		
44	295-17-0	Cyclotetradecane		
44	2958-76-1	Decahydro-2-methylnaphthalene		
44	29799-19-7	Cyclohexane, 1-(1,5-dimethylhexyl)-4-methyl-		
44	2980-69-0	4-Methylundecane		
44	3031-15-0	1,2,3,4-Tetramethylnaphthalene		
44	30316-17-7	1,2,3,4-Tetrahydro-2,5,8-trimethylnaphthalene		
44	30654-45-6	Naphthalene, 6-butyl-1,2,3,4-tetrahydro-		
44	31295-56-4	2,6,11-Trimethyldodecane		
44	3178-23-2	Dicyclohexylmethane		
44	32367-54-7	Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-		
44	3333-52-6	Tetramethylsuccinonitrile		
44	334-48-5	Decanoic acid		
44	34303-81-6	3-Hexadecene, (Z)-		
44	35216-11-6	7-Tetradecyne		
44	35365-59-4	9-Octadecyne		
44	3777-69-3	2-Pentylfuran		
44	3877-19-8	Naphthalene, 1,2,3,4-tetrahydro-2-methyl-		
44	3891-98-3	2,6,10-Trimethyldodecane		
44	3892-00-0	2,6,10-Trimethylpentadecane		
44	4032-93-3	heptane, 2,3,6-trimethyl-		
44	40650-41-7	1,1,5-Trimethylindan		
44	4132-72-3	Benzene, 1,4-dimethyl-2-(1-methylethyl)-		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
44	41446-57-5	3-Tridecene, (3E)-		
44	41446-59-7	2-tridecene, (z)-		
44	41446-60-0	7-Tetradecene, (Z)-		
44	41446-65-5	4-Tetradecene, (Z)-		
44	41446-66-6	5-tetradecene, (e)-		
44	41446-68-8	3-Tetradecene, (E)-		
44	41446-78-0	4-Tetradecene, (4E)-		
44	4175-53-5	1H-Indene, 2,3-dihydro-1,3-dimethyl-		
44	4175-54-6	Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-		
44	41977-45-1	Bicyclo[4.1.0]heptane, 7-pentyl-		
44	41977-48-4	bicyclo[4.1.0]heptane, 3-methyl-7-pentyl-		
44	4218-48-8	Benzene, 1-ethyl-4-(1-methylethyl)-		
44	42775-75-7	naphthalene, 5-ethyl-1,2,3,4-tetrahydro-		
44	42775-77-9	6-n-Propyltetralin		
44	4291-79-6	1-Methyl-2-propyl-cyclohexane		
44	4292-75-5	Hexylcyclohexane		
44	4292-92-6	Pentylcyclohexane		
44	4359-46-0	1,3-Dioxolane, 2-ethyl-4-methyl-		
44	4413-16-5	Benzene, (1-cyclohexylethyl)-		
44	4413-21-2	1,1-Dicyclopentylethane		
44	4431-89-4	(Cyclopentylmethyl)cyclohexane		
44	4457-00-5	Cyclopentane, hexyl-		
44	4701-36-4	Benzene, (1-ethyl-1-propenyl)-		
44	4706-90-5	1,3-Dimethyl-5-isopropylbenzene		
44	475-03-6	1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene		
44	480-72-8	Acenaphthylene, 1,2,2a,3,4,5-hexahydro-		
44	490-65-3	1-Methyl-7-isopropyl-naphthalene		
44	4912-92-9	1,1-Dimethylindan		
44	4920-99-4	Benzene, 1-ethyl-3-(1-methylethyl)-		
44	493-02-7	Naphthalene, decahydro-, trans-		
44	503-74-2	Isovaleric acid		
44	506-43-4	(Z,Z)-9,12-Octadecadien-1-ol		
44	50991-08-7	1,1'-Bicyclohexyl, 2-methyl-, cis-		
44	50991-09-8	1,1'-Bicyclohexyl, 2-methyl-, trans-		
44	50991-12-3	1,1'-Bicyclohexyl, 2-ethyl-, cis-		
44	50991-13-4	1,1'-Bicyclohexyl, 2-ethyl-, trans-		
44	526-73-8	1,2,3-Trimethylbenzene		
44	52845-07-5	Isoeicosane		
44	52914-66-6	Cyclopentadecanone, 2-methyl-		
44	529-34-0	1,2,3,4-Tetrahydronaphthalen-1-one		
44	53485-49-7	Tricyclo[6.4.0.0(2,7)]dodecane		
44	53535-33-4	Heptanol		
44	535-77-3	m-Cymene		
44	538-68-1	Pentylbenzene		
44	538-86-3	Benzyl methyl ether		
44	5402-53-9	Chloromethyl propanoate		
44	54105-66-7	Undecylcyclohexane		
44	54105-77-0	(2-methylbutyl)cyclohexane		
44	542-28-9	Tetrahydro-2H-pyran-2-one		
44	54290-12-9	7-heptadecene		
44	54410-74-1	1-Methyl-2-(1-ethylpropyl)benzene		
44	54411-00-6	cyclohexane, 1-methyl-4-(1-methylbutyl)-		
44	54411-01-7	1-Methyl-2-pentylcyclohexane		
44	544-25-2	1,3,5-Cycloheptatriene		
44	544-63-8	Tetradecanoic acid		
44	544-76-3	Hexadecane		
44	54676-39-0	2-BUTYL-1,1,3-TRIMETHYL-CYCLOHEXANE		
44	54766-91-5	Bicyclo[10.1.0]tridec-1-ene		
44	54823-97-1	cis-1-(Cyclohexylmethyl)-4-methylcyclohexane		
44	54823-98-2	Cyclohexane, 1-(cyclohexylmethyl)-4-methyl-, trans-		
44	54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-		
44	54965-05-8	Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-		
44	55030-62-1	Tridecane, 4,8-dimethyl-		
44	5557-93-7	Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-		
44	556-67-2	Octamethylcyclotetrasiloxane		
44	55669-88-0	1-Isobutyl-2,5-dimethylbenzene		
44	55682-81-0	3-tert-Butyl-1,2-dihydronaphthalene		
44	56325-56-5	Cyclodecene, 3-bromo-		
44	565-67-3	3-Pentanol, 2-methyl-		
44	57-10-3	Hexadecanoic acid		
44	5743-97-5	phenanthrene, tetradecahydro-		
44	581-40-8	2,3-Dimethylnaphthalene		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
44	581-42-0	2,6-Dimethylnaphthalene		
44	58175-57-8	1-Pentanol, 2-propyl-		
44	584-02-1	3-Pentanol		
44	5842-53-5	2,2,4-Trimethylpent-3-en-1-ol		
44	589-98-0	3-octanol		
44	591-11-7	2(5H)-Furanone, 5-methyl-		
44	592-27-8	2-Methylheptane		
44	593-45-3	Octadecane		
44	593-49-7	Heptacosane		
44	594-61-6	2-Hydroxyisobutyric acid		
44	597-49-9	3-Pentanol, 3-ethyl-		
44	6006-33-3	Cyclohexane, tridecyl-		
44	60212-33-1	4-Tetradecyne		
44	60274-60-4	Pentane, 1-chloro-5-iodo-		
44	6044-71-9	Dodecane, 6-methyl-		
44	605-39-0	1,1'-Biphenyl, 2,2'-dimethyl-		
44	61142-19-6	(1,3-Dimethylbutyl)cyclohexane		
44	61142-38-9	Cyclohexane, (3-methylpentyl)-		
44	61142-66-3	cyclopentene, 5-hexyl-3,3-dimethyl-		
44	61142-68-5	1-Hexyl-3-methylcyclopentane		
44	61142-70-9	2,4-Diethyl-1-methylcyclohexane		
44	6117-97-1	4-Methyldodecane		
44	61208-94-4	Cyclohexane, (1-methylbutyl)-		
44	61233-71-4	1,6,9-tetradecatriene		
44	613-33-2	4,4'-Dimethylbiphenyl		
44	61413-70-5	Chloromethyl octanoate		
44	6165-44-2	Cyclohexane, 1,1'-(1,4-butanediyl)bis-		
44	61886-62-2	3-Hexadecyne		
44	620-14-4	3-Ethyltoluene		
44	62016-19-7	octane, 6-ethyl-2-methyl-		
44	62016-28-8	2,2,6-Trimethyloctane		
44	62016-37-9	2,4,6-Trimethyloctane		
44	62108-21-8	Decane, 6-ethyl-2-methyl-		
44	62183-55-5	3-Ethyl-2,7-dimethyloctane		
44	62199-51-3	1-Pentyl-2-propylcyclopentane		
44	62199-52-4	1,2-Dibutylcyclopentane		
44	62238-29-3	cyclohexane, 1-ethyl-1,3-dimethyl-, trans-		
44	62238-33-9	cyclohexane, 1-ethyl-2-propyl-		
44	623-55-2	3-Hexanol, 5-methyl-		
44	625-31-0	4-Penten-2-ol		
44	626-98-2	2-Pentenoic acid		
44	629-50-5	Tridecane		
44	629-59-4	Tetradecane		
44	629-62-9	Pentadecane		
44	629-78-7	Heptadecane		
44	629-89-0	Octadecyne		
44	629-92-5	Nonadecane		
44	6305-52-8	2-n-Butyldecahydronaphthalene		
44	638-29-9	Valeryl chloride		
44	638-36-8	2,6,10,14-Tetramethylhexadecane		
44	638-60-8	2-Tetradecene		
44	6418-41-3	tridecane, 3-methyl-		
44	6418-44-6	heptadecane, 3-methyl-		
44	643-93-6	3-Methylbiphenyl		
44	645-10-3	1,7-dimethyl-4-(1-methylethyl)cyclodecane		
44	65-85-0	Benzoic acid		
44	66-25-1	Hexanal		
44	66542-51-6	Chloromethyl hexanoate		
44	66552-62-3	Naphthalene, decahydro-1,5-dimethyl-		
44	66660-42-2	cis, cis-3-ethylbicyclo[4.4.0]decane		
44	6682-71-9	4,7-Dimethylindan		
44	6750-34-1	1-dodecanol, 3,7,11-trimethyl-		
44	68603-15-6	Alcohols, C6-12		
44	695-06-7	gamma-Caprolactone		
44	6975-98-0	2-Methyldecane		
44	6982-25-8	DL-2,3-Butanediol		
44	698-76-0	delta-Octanolactone		
44	700000-97-1	2,3,3-Trimethyl-1-hexene		
44	700-12-9	Benzene, pentamethyl-		
44	702-79-4	1,3-Dimethyladamantane		
44	7045-71-8	2-Methylundecane		
44	705-86-2	6-Pentyltetrahydro-2H-pyran-2-one		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
44	706-14-9	gamma-Decanolactone		
44	707-35-7	1,3,5-Trimethyladamantane		
44	7206-14-6	3-Dodecene, (E)-		
44	7206-19-1	3-Octadecene, (E)-		
44	7206-25-9	9-octadecene, (e)-		
44	72218-58-7	3-Methylheptyl acetate		
44	73105-67-6	1-Iodo-2-methylundecane		
44	7326-46-7	2-Furanol, tetrahydro-2-methyl-		
44	74054-92-5	1,1,6,6-tetramethylspiro[4.4]nonane		
44	74367-34-3	3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate		
44	74646-37-0	1-Tridecyn-4-ol		
44	764-96-5	(5Z)-5-Undecene		
44	767-58-8	Indan, 1-methyl-		
44	77877-94-2	Chloromethyl pentanoate		
44	78-67-1	Azobisisobutyronitrile		
44	79273-13-5	dispiro[4.2.4.2]tetradecane		
44	79-31-2	2-Methylpropanoic acid		
44	80625-32-7	1,e-8,z-10-pentadecatriene		
44	80655-44-3	Decahydro-4,4,8,9,10-pentamethylnaphthalene		
44	821-55-6	2-Nonanone		
44	823-22-3	2H-Pyran-2-one, tetrahydro-6-methyl-		
44	825-51-4	2-Naphthalenol, decahydro-		
44	826-18-6	Benzene, 1-pentenyl-		
44	827-52-1	Cyclohexylbenzene		
44	83-33-0	1H-Inden-1-one, 2,3-dihydro-		
44	84-69-5	Diisobutyl phthalate		
44	84-74-2	Dibutyl phthalate		
44	871-83-0	2-Methylnonane		
44	87-41-2	Phthalide		
44	874-35-1	5-Methylindan		
44	877-44-1	1,2,4-Triethylbenzene		
44	91-20-3	Naphthalene		
44	91531-54-3	1,1,3a-trimethyl-1a,3a,5,6-tetrahydro-1h-cyclopropa[c]pentalen-4-one		
44	91-57-6	2-Methylnaphthalene		
44	92013-16-6	1H-Indene, 2,3-dihydro-4-propyl-		
44	92-51-3	Dicyclohexyl		
44	93-53-8	Hydratropaldehyde		
44	93-55-0	1-Phenylpropan-1-one		
44	939-27-5	2-Ethyl-naphthalene		
44	95-16-9	Benzothiazole		
44	959028-24-1	4-Ethyl-2,3-dimethylhex-2-ene		
44	95-93-2	1,2,4,5-Tetramethylbenzene		
44	98-54-4	4-tert-Butylphenol		
44	98-82-8	Cumene		
44	98-86-2	Acetophenone		
44	99328-46-8	5-Methyl-1-hepten-4-ol		
44	99-87-6	p-Cymene		
45	7440-09-7	Potassium	515	mg/L
45	14127-61-8	Calcium ion	4810	mg/L
45	14808-79-8	Sulfate	2420	mg/L
45	16887-00-6	Chloride	56200	mg/L
45	24959-67-9	Bromide	292	mg/L
45	71-52-3	Bicarbonate	495	mg/L
45	7439-95-4	Magnesium	1500	mg/L
45	7440-24-6	Strontium	108	mg/L
46	14808-79-8	Sulfate	69.1632	mg/L
46	15035-72-0	Hydrosulfide	102.517	mg/L
46	71-50-1	Acetate	312.9385	mg/L
46	72-03-7	Propanoate	31.42096	mg/L
47	7429-90-5	Aluminum	1.817206618	mg/L
47	7439-89-6	Iron	0.46183815	mg/L
47	7439-96-5	Manganese	0.065376272	mg/L
47	7439-98-7	Molybdenum	0.0028785	mg/L
47	7440-38-2	Arsenic	0.009739807	mg/L
47	7440-39-3	Barium	0.61385169	mg/L
47	7440-42-8	Boron	0.164312	mg/L
47	7440-47-3	Chromium	0.011959103	mg/L
47	7440-50-8	Copper	0.01969926	mg/L
47	7440-66-6	Zinc	0.0183064	mg/L
47	7782-49-2	Selenium	0.00236913	mg/L
48	7440-09-7	Potassium	363	mg/L
48	14127-61-8	Calcium ion	2935	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
48	14808-79-8	Sulfate	12.9	mg/L
48	16887-00-6	Chloride	28500	mg/L
48	17341-25-2	Sodium ion	12200	mg/L
48	24959-67-9	Bromide	19	mg/L
48	7429-90-5	Aluminum	105	mg/L
48	7439-95-4	Magnesium	104	mg/L
48	7440-24-6	Strontium	591	mg/L
48	7440-39-3	Barium	697	mg/L
49	100-41-4	Ethylbenzene	7.34	mg/L
49	100-42-5	Styrene	52	mg/L
49	108-88-3	Toluene	27.3	mg/L
49	111-76-2	2-Butoxyethanol	77.5	mg/L
49	179601-23-1	m,p-Xylene	40.1	mg/L
49	2682-20-4	2-Methyl-3(2H)-isothiazolone	9.51	mg/L
49	68-12-2	N,N-Dimethylformamide	519	mg/L
49	71-43-2	Benzene	4.56	mg/L
49	79-06-1	Acrylamide	99.2	mg/L
49	91-20-3	Naphthalene	3.54	mg/L
49	95-47-6	o-Xylene	15	mg/L
49	95-63-6	1,2,4-Trimethylbenzene	78.5	mg/L
49	98-82-8	Cumene	4.21	mg/L
50	100-41-4	Ethylbenzene	399.84	mg/L
50	103-65-1	Propylbenzene		
50	106-42-3	p-Xylene	0.46	mg/L
50	1074-43-7	1-Methyl-3-propylbenzene		
50	108-88-3	Toluene	5.61	mg/L
50	108-90-7	Chlorobenzene	0.35	mg/L
50	109-66-0	Pentane		
50	109-74-0	Butanenitrile		
50	1768-36-1	Propyl cyanate		
50	19261-13-3	1-(2-Furanyl)-3-butene-1,2-diol		
50	2406-25-9	Di-tert-butyl nitroxide		
50	25414-22-6	2-Methoxyfuran		
50	2717-39-7	1,4,5,8-Tetramethylnaphthalene		
50	5618-62-2	O-Isobutylhydroxylamine		
50	591-48-0	3-Methylcyclohexene		
50	71312-54-4	1,4-Dimethyl-2,3-diazabicyclo[2.2.1]hept-2-ene		
50	71-43-2	Benzene	778.51	mg/L
50	85-01-8	Phenanthrene		
50	89-74-7	1-(2,4-Dimethylphenyl)ethanone		
50	91-57-6	2-Methylnaphthalene		
50	96-04-8	2,3-Heptanedione		
51	7440-09-7	Potassium	10700	mg/L
51	7783-06-4	Hydrogen sulfide	125	mg/L
51	14808-79-8	Sulfate	197	mg/L
51	16887-00-6	Chloride	201000	mg/L
51	16984-48-8	Fluoride	11.8	mg/L
51	24959-67-9	Bromide	2190	mg/L
51	461-55-2	Butyrate	3	mg/L
51	71-50-1	Acetate	264	mg/L
51	72-03-7	Propanoate	31	mg/L
51	7429-90-5	Aluminum	0.367	mg/L
51	7439-89-6	Iron	465	mg/L
51	7439-92-1	Lead	70.2	mg/L
51	7439-93-2	Lithium	74	mg/L
51	7439-95-4	Magnesium	6180	mg/L
51	7439-96-5	Manganese	212	mg/L
51	7440-17-7	Rubidium	19.6	mg/L
51	7440-23-5	Sodium	69300	mg/L
51	7440-24-6	Strontium	1940	mg/L
51	7440-39-3	Barium	196	mg/L
51	7440-42-8	Boron	692	mg/L
51	7440-43-9	Cadmium	0.99	mg/L
51	7440-46-2	Cesium	2.6	mg/L
51	7440-50-8	Copper	0.061	mg/L
51	7440-66-6	Zinc	243	mg/L
51	7440-70-2	Calcium	48600	mg/L
51	7553-56-2	Iodine	106	mg/L
51	7631-86-9	Silica	53	mg/L
51	7664-41-7	Ammonia	119	mg/L
51	79-31-2	2-Methylpropanoic acid	4	mg/L
52	7440-09-7	Potassium	99	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
52	103-65-1	Propylbenzene	0.00051	mg/L
52	108-10-1	4-Methyl-2-pentanone	0.04	mg/L
52	108-67-8	1,3,5-Trimethylbenzene	0.023	mg/L
52	14808-79-8	Sulfate	560	mg/L
52	16887-00-6	Chloride	16000	mg/L
52	17341-25-2	Sodium ion	10000	mg/L
52	24959-67-9	Bromide	260	mg/L
52	7439-95-4	Magnesium	200	mg/L
52	7440-70-2	Calcium	1000	mg/L
52	75-09-2	Dichloromethane	0.0026	mg/L
52	75-65-0	tert-Butyl alcohol	0.071	mg/L
52	78-93-3	Methyl ethyl ketone	0.098	mg/L
52	95-47-6	o-Xylene	0.003	mg/L
52	95-63-6	1,2,4-Trimethylbenzene	0.002	mg/L
52	98-82-8	Cumene	0.00054	mg/L
53	7440-09-7	Potassium		
53	14808-79-8	Sulfate		
53	16887-00-6	Chloride		
53	3812-32-6	Carbonate		
53	71-52-3	Bicarbonate		
53	7429-90-5	Aluminum		
53	7439-89-6	Iron		
53	7439-95-4	Magnesium		
53	7440-21-3	Silicon		
53	7440-23-5	Sodium		
53	7440-24-6	Strontium		
53	7440-39-3	Barium		
53	7440-42-8	Boron		
53	7440-67-7	Zirconium		
53	7440-70-2	Calcium		
54	7440-09-7	Potassium	183.992	mg/L
54	14127-61-8	Calcium ion	2344.824476	mg/L
54	14808-79-8	Sulfate	10.71666667	mg/L
54	15438-31-0	Fe +2 ion	83.89098657	mg/L
54	16887-00-6	Chloride	58540	mg/L
54	17341-25-2	Sodium ion	28049.04918	mg/L
54	24959-67-9	Bromide	292.0182728	mg/L
54	7439-95-4	Magnesium	1911.606746	mg/L
55	16887-00-6	Chloride	9794	mg/L
55	17341-25-2	Sodium ion	4106	mg/L
56	14798-03-9	Ammonium	1469	mg/L
56	14808-79-8	Sulfate	131	mg/L
56	16887-00-6	Chloride	88457	mg/L
56	24959-67-9	Bromide	409	mg/L
56	71-52-3	Bicarbonate	353	mg/L
56	7429-90-5	Aluminum	0.612	mg/L
56	7439-89-6	Iron	18.097	mg/L
56	7439-92-1	Lead	1.047	mg/L
56	7439-93-2	Lithium	22.779	mg/L
56	7439-95-4	Magnesium	790	mg/L
56	7439-96-5	Manganese	11.464	mg/L
56	7440-02-0	Nickel	0.497	mg/L
56	7440-17-7	Rubidium	8.111	mg/L
56	7440-23-5	Sodium	38701	mg/L
56	7440-24-6	Strontium	582	mg/L
56	7440-28-0	Thallium	0.134	mg/L
56	7440-39-3	Barium	13.563	mg/L
56	7440-42-8	Boron	163.298	mg/L
56	7440-43-9	Cadmium	0.019	mg/L
56	7440-48-4	Cobalt	0.105	mg/L
56	7440-50-8	Copper	0.127	mg/L
56	7440-62-2	Vanadium	0.683	mg/L
56	7440-66-6	Zinc	8.36	mg/L
56	7440-70-2	Calcium	9081	mg/L
56	7782-49-2	Selenium	0.65	mg/L
57	7440-09-7	Potassium	101.3	mg/L
57	105-67-9	2,4-Dimethylphenol	0.79	mg/L
57	107-92-6	Butanoic acid	19	mg/L
57	108-95-2	Phenol	0.83	mg/L
57	117-81-7	Di(2-ethylhexyl) phthalate	0.029	mg/L
57	123-91-1	1,4-Dioxane	0.06	mg/L
57	129-00-0	Pyrene	0.0009	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
57	131-11-3	Dimethyl phthalate	0.015	mg/L
57	1319-77-3	Cresol	0.17	mg/L
57	1330-20-7	Xylenes	0.03	mg/L
57	14797-55-8	Nitrate	5.2	mg/L
57	14808-79-8	Sulfate	1.3	mg/L
57	16887-00-6	Chloride	13600	mg/L
57	18496-25-8	Sulfide	0.31	mg/L
57	24959-67-9	Bromide	87.2	mg/L
57	57-12-5	Cyanide	0.055	mg/L
57	64-19-7	Acetic acid	1600	mg/L
57	67-64-1	Acetone	16	mg/L
57	68140-01-2	N-[3-(Dimethylamino)propyl] coco amides		
57	71060-57-6	Oxanol KD-6		
57	7429-90-5	Aluminum	0.064	mg/L
57	7439-89-6	Iron	81.42	mg/L
57	7439-93-2	Lithium	3.519	mg/L
57	7439-95-4	Magnesium	106.4	mg/L
57	7439-96-5	Manganese	1.471	mg/L
57	7440-02-0	Nickel	0.042	mg/L
57	7440-17-7	Rubidium	0.23	mg/L
57	7440-21-3	Silicon	19.65	mg/L
57	7440-23-5	Sodium	6943.9	mg/L
57	7440-24-6	Strontium	60.25	mg/L
57	7440-32-6	Titanium	0.028	mg/L
57	7440-38-2	Arsenic	0.067	mg/L
57	7440-39-3	Barium	8.542	mg/L
57	7440-42-8	Boron	3.105	mg/L
57	7440-46-2	Cesium	0.073	mg/L
57	7440-47-3	Chromium	0.058	mg/L
57	7440-50-8	Copper	0.288	mg/L
57	7440-62-2	Vanadium	0.12	mg/L
57	7440-66-6	Zinc	0.051	mg/L
57	7440-70-2	Calcium	524.1	mg/L
57	7664-41-7	Ammonia	24.7	mg/L
57	78-93-3	Methyl ethyl ketone	0.24	mg/L
57	79-09-4	Propionic acid	33	mg/L
57	85-01-8	Phenanthrene	0.003	mg/L
57	85-68-7	Benzyl butyl phthalate	0.0042	mg/L
57	91-57-6	2-Methylnaphthalene	0.004	mg/L
57	95-48-7	o-Cresol	0.15	mg/L
58	14127-61-8	Calcium ion	435	mg/L
58	14808-79-8	Sulfate	446	mg/L
58	16887-00-6	Chloride	15712	mg/L
58	17341-25-2	Sodium ion	10199	mg/L
58	71-52-3	Bicarbonate	3660	mg/L
58	7429-90-5	Aluminum	16	mg/L
58	7439-89-6	Iron	171.1	mg/L
58	7439-95-4	Magnesium	57.7	mg/L
58	7440-24-6	Strontium	60.4	mg/L
58	7440-39-3	Barium	15.5	mg/L
58	7440-66-6	Zinc	6.7	mg/L
59	7440-09-7	Potassium	10300	mg/L
59	14808-79-8	Sulfate	9164	mg/L
59	16887-00-6	Chloride	48586	mg/L
59	3812-32-6	Carbonate	35.92	mg/L
59	71-52-3	Bicarbonate	1342	mg/L
59	7439-89-6	Iron	1744	mg/L
59	7439-95-4	Magnesium	313	mg/L
59	7439-96-5	Manganese	824.56	mg/L
59	7440-23-5	Sodium	115205	mg/L
59	7440-39-3	Barium	897	mg/L
59	7440-42-8	Boron	18.7	mg/L
59	7440-70-2	Calcium	1325	mg/L
60	14383-50-7	Thiosulfate	19.05989	mg/L
60	14808-79-8	Sulfate	185.3958	mg/L
60	15438-31-0	Fe +2 ion	656.72544	mg/L
60	16887-00-6	Chloride	117000	mg/L
60	18496-25-8	Sulfide	8.015	mg/L
60	71-50-1	Acetate	10037.65	mg/L
61	16887-00-6	Chloride	147436.3	mg/L
61	7440-23-5	Sodium	102715.6	mg/L
61	7440-39-3	Barium	7094.5	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
61	7440-70-2	Calcium	31668.3	mg/L
62	111-76-2	2-Butoxyethanol		
63	1849-76-9	3-bromo-5-chloro-4-hydroxybenzaldehyde		
63	3147-55-5	Benzoic acid, 3,5-dibromo-2-hydroxy-		
63	53715-09-6	Chloro(iodo)acetic acid		
63	598-89-0	Diiodoacetic acid		
63	6937-34-4	3-iodophthalic acid		
64	7440-09-7	Potassium	48	mg/L
64	14797-55-8	Nitrate	39	mg/L
64	14808-79-8	Sulfate	21	mg/L
64	16887-00-6	Chloride	7065	mg/L
64	3812-32-6	Carbonate	341	mg/L
64	71-52-3	Bicarbonate	1396	mg/L
64	7439-89-6	Iron	0.2	mg/L
64	7439-95-4	Magnesium	50	mg/L
64	7440-23-5	Sodium	5111	mg/L
64	7440-42-8	Boron	30	mg/L
64	7440-50-8	Copper	0.03	mg/L
64	7440-66-6	Zinc	0.06	mg/L
64	7440-70-2	Calcium	8	mg/L
65	123-86-4	Butyl acetate	0.9	mg/L
65	50-00-0	Formaldehyde	0.8	mg/L
65	67-64-1	Acetone	2.4	mg/L
65	71-36-3	1-Butanol	16.5	mg/L
65	75-07-0	Acetaldehyde	0.1	mg/L
65	91-20-3	Naphthalene	88.4	mg/L
66	16887-00-6	Chloride	160588.5	mg/L
66	7439-93-2	Lithium	274.13	mg/L
67	2207-01-4	(Z)-1,2-Dimethylcyclohexane		
67	4810-09-7	3-Methyl-1-heptene		
67	5911-04-6	3-Methylnonane		
67	100-41-4	Ethylbenzene		
67	1008-80-6	2,3-Dimethyldecahydronaphthalene		
67	103-65-1	Propylbenzene		
67	1072-05-5	2,6-Dimethylheptane		
67	1074-43-7	1-Methyl-3-propylbenzene		
67	107-83-5	2-Methylpentane		
67	108-38-3	m-Xylene		
67	108-67-8	1,3,5-Trimethylbenzene		
67	108-87-2	Methylcyclohexane		
67	108-88-3	Toluene		
67	110-54-3	n-Hexane		
67	111-65-9	Octane		
67	111-67-1	2-Octene		
67	111-84-2	Nonane		
67	1120-21-4	Undecane		
67	112-40-3	Dodecane		
67	112-41-4	1-Dodecene		
67	112-88-9	1-Octadecene		
67	112-89-0	1-Bromooctadecane		
67	112-95-8	Eicosane		
67	117-81-7	Di(2-ethylhexyl) phthalate		
67	1192-18-3	(Z)-1,2-Dimethylcyclopentane		
67	119736-96-8	1',4'-Dihydroxy-7'-methoxy-2,3'-dimethyl-(-)-[1,2'-binaphthalene]-5,5',8,8'-tetrone		
67	123-79-5	Diocetyl hexanedioate		
67	124-18-5	Decane		
67	13150-81-7	2,6-Dimethyldecane		
67	13151-34-3	3-Methyldecane		
67	13151-35-4	5-Methyldecane		
67	13287-21-3	6-Methyltridecane		
67	13287-24-6	9-Methylnonadecane		
67	14113-60-1	rel-(1R,2S)-1,2-Diethylcyclohexadecane		
67	142-82-5	Heptane		
67	1560-93-6	2-Methylpentadecane		
67	1560-95-8	2-Methyltetradecane		
67	1560-96-9	2-Methyltridecane		
67	1560-97-0	2-Methyldodecane		
67	15869-86-0	4-Ethyldecane		
67	15869-93-9	3,5-Dimethyloctane		
67	1630-94-0	1,1-Dimethylcyclopropane		
67	1640-89-7	Ethylcyclopentane		
67	1678-91-7	Ethylcyclohexane		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
67	1678-92-8	Propylcyclohexane		
67	1678-93-9	Butylcyclohexane		
67	17301-23-4	2,6-Dimethylundecane		
67	17301-27-8	2,10-Dimethylundecane		
67	17301-28-9	3,6-Dimethylundecane		
67	17301-94-9	4-Methylnonane		
67	17302-32-8	3,7-Dimethylnonane		
67	17312-55-9	3,8-Dimethyldecane		
67	17312-80-0	2,4-Dimethylundecane		
67	1786-12-5	1,7,11-Trimethyl-4-(1-methylethyl)cyclotetradecane		
67	1795-16-0	Decylcyclohexane		
67	1839-63-0	1,3,5-Trimethylcyclohexane		
67	18435-45-5	1-Nonadecene		
67	18835-32-0	1-Tricosene		
67	1921-70-6	Norphytane		
67	2040-96-2	Propylcyclopentane		
67	2051-30-1	2,6-Dimethyloctane		
67	20524-86-1	Bis(dichloromethyl) ether		
67	2131-41-1	1,4,5-Trimethylnaphthalene		
67	2131-42-2	1,4,6-Trimethylnaphthalene		
67	21693-55-0	1,5,7-Trimethyl-1,2,3,4-tetrahydronaphthalene		
67	2213-23-2	2,4-Dimethylheptane		
67	2216-33-3	3-Methyloctane		
67	2234-75-5	1,2,4-Trimethylcyclohexane		
67	2245-38-7	1,6,7-Trimethylnaphthalene		
67	2385-77-5	(3R)-3,7-Dimethyloct-6-enal		
67	24145-88-8	(E)-1,4-Dimethyladamantane		
67	24145-89-9	(Z)-1,4-Dimethyladamantane		
67	2453-00-1	1,3-Dimethylcyclopentane		
67	2471-83-2	1-Ethylidene-1H-indene		
67	2471-84-3	1-Methylene-1H-indene		
67	25117-24-2	4-Methyltetradecane		
67	25117-32-2	5-Methyltetradecane		
67	2531-84-2	2-Methylphenanthrene		
67	26730-12-1	4-Methyltridecane		
67	26730-14-3	7-Methyltridecane		
67	26761-40-0	Diisodecyl phthalate		
67	27554-26-3	Diisooctyl phthalate		
67	2815-57-8	1,2,3-Trimethylcyclopentane		
67	2815-58-9	1,2,4-Trimethylcyclopentane		
67	2847-72-5	4-Methyldecane		
67	2855-19-8	1,2-Epoxydodecane		
67	2885-00-9	1-Octadecanethiol		
67	295-02-3	Cyclotridecane		
67	295-17-0	Cyclotetradecane		
67	295-48-7	Cyclopentadecane		
67	2958-76-1	Decahydro-2-methylnaphthalene		
67	297-35-8	Cyclotriacontane		
67	2980-69-0	4-Methylundecane		
67	3073-66-3	1,1,3-Trimethylcyclohexane		
67	3074-71-3	2,3-Dimethylheptane		
67	31295-56-4	2,6,11-Trimethyldodecane		
67	3221-61-2	2-Methyloctane		
67	3386-33-2	Octadecyl chloride		
67	3726-46-3	1-Ethyl-2-methylcyclopentane		
67	3728-54-9	1-Ethyl-2-methylcyclohexane		
67	3728-55-0	1-Ethyl-3-methylcyclohexane		
67	3728-56-1	1-Ethyl-4-methylcyclohexane		
67	38274-72-5	(Z)-4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane		
67	3891-98-3	2,6,10-Trimethyldodecane		
67	3892-00-0	2,6,10-Trimethylpentadecane		
67	40710-32-5	Nonahexacontanoic acid		
67	4291-79-6	1-Methyl-2-propyl-cyclohexane		
67	4292-75-5	Hexylcyclohexane		
67	4292-92-6	Pentylcyclohexane		
67	4306-65-4	1,1,3,5-Tetramethylcyclohexane		
67	442662-72-8	2-Ethyl-1,1,3-trimethylcyclohexane		
67	4453-90-1	1,4-Dihydro-1,4-methanonaphthalene		
67	4461-48-7	4-Methyl-2-pentene		
67	51050-50-1	2-Methyl-7-octadecene		
67	513-35-9	2-Methyl-2-butene		
67	526-73-8	1,2,3-Trimethylbenzene		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
67	53172-84-2	(1-Methyl-1-buten-1-yl)benzene		
67	541-91-3	3-Methylcyclopentadecan-1-one		
67	54411-01-7	1-Methyl-2-pentylcyclohexane		
67	544-76-3	Hexadecane		
67	544-85-4	Dotriacontane		
67	54833-23-7	10-Methylcosane		
67	55282-11-6	11-Pentan-3-ylheneicosane		
67	55282-68-3	2'-Dodecyl- 1,1':3',1''-tercyclopentane		
67	55821-04-0	syn-1,6:8,13-Bismethano[14]annulene		
67	56009-20-2	1-(1,5-Dimethylhexyl)-4-(4-methylpentyl)cyclohexane		
67	56221-91-1	13-Tetradecen-1-yl acetate		
67	56292-65-0	2,5-Dimethyldodecane		
67	563-46-2	2-Methylbut-1-ene		
67	571-58-4	1,4-Dimethylnaphthalene		
67	571-61-9	1,5-Dimethylnaphthalene		
67	575-43-9	1,6-Dimethylnaphthalene		
67	581-40-8	2,3-Dimethylnaphthalene		
67	581-42-0	2,6-Dimethylnaphthalene		
67	582-16-1	2,7-Dimethylnaphthalene		
67	589-43-5	2,4-Dimethylhexane		
67	589-53-7	4-Methylheptane		
67	589-90-2	1,4-Dimethylcyclohexane		
67	590-66-9	1,1-Dimethylcyclohexane		
67	591-21-9	1,3-Dimethylcyclohexane		
67	592-27-8	2-Methylheptane		
67	593-45-3	Octadecane		
67	593-49-7	Heptacosane		
67	611-14-3	1-Ethyl-2-methylbenzene		
67	61141-72-8	4,6-Dimethyldodecane		
67	61142-52-7	1-Butyl-2-pentylcyclopentane		
67	6165-40-8	7-Methylpentadecane		
67	619-99-8	3-Ethylhexane		
67	620-14-4	3-Ethyltoluene		
67	62016-79-9	1-Chloroheptacosane		
67	62199-51-3	1-Pentyl-2-propylcyclopentane		
67	629-50-5	Tridecane		
67	629-59-4	Tetradecane		
67	629-62-9	Pentadecane		
67	629-72-1	1-Bromopentadecane		
67	629-78-7	Heptadecane		
67	629-92-5	Nonadecane		
67	629-94-7	Heneicosane		
67	629-97-0	Docosane		
67	629-99-2	Pentacosane		
67	630-01-3	Hexacosane		
67	630-02-4	Octacosane		
67	630-03-5	Nonacosane		
67	630-06-8	Hexatriacontane		
67	630-07-9	Pentatriacontane		
67	638-36-8	2,6,10,14-Tetramethylhexadecane		
67	638-67-5	Tricosane		
67	638-68-6	Triacotane		
67	64275-73-6	(Z)-5-Octen-1-ol		
67	646-31-1	Tetracosane		
67	66826-95-7	1-(Cyclohexylmethyl)-4-methylcyclohexane		
67	67-64-1	Acetone		
67	6765-39-5	1-Heptadecene		
67	67-66-3	Chloroform		
67	69586-09-0	2,2-Dichloro-3,6-dimethyl-2H-1,2-oxasiline		
67	6971-40-0	17-pentatriacontene		
67	6975-98-0	2-Methyldecane		
67	7045-71-8	2-Methylundecane		
67	7098-21-7	Tritetracontane		
67	7098-22-8	Tetratetracontane		
67	73105-67-6	1-Iodo-2-methylundecane		
67	7320-37-8	1,2-Epoxyhexadecane		
67	74646-31-4	14-Bromo-1-tetradecene		
67	75-09-2	Dichloromethane		
67	75-34-3	1,1-Dichloroethane		
67	7773-83-3	1-Docosanethiol		
67	779-02-2	9-Methylantracene		
67	77-90-7	Acetyl tributyl citrate		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
67	829-26-5	2,3,6-Trimethylnaphthalene		
67	84-77-5	Didecyl phthalate		
67	852228-22-9	1,54-Dibromotetrapentacotane		
67	866760-27-2	(4Z)-2-Methyl-4-tetradecene		
67	871-83-0	2-Methylnonane		
67	89-16-7	Bis(8-methylnonyl) phthalate		
67	89-18-9	Butyl 8-methylnonyl phthalate		
67	90-12-0	1-Methylnaphthalene		
67	90548-09-7	Decahydro-1-methyl-2-methylenenaphthalene		
67	912629-93-7	(9E)-8-Methyl-9-tetradecen-1-yl acetate		
67	91-57-6	2-Methylnaphthalene		
67	930-89-2	(Z)-1-Ethyl-2-methylcyclopentane		
67	933-98-2	1-Ethyl-2,3-dimethylbenzene		
67	934-80-5	1,2-Dimethyl-4-ethylbenzene		
67	938-06-7	(4aS,8aR)-4a-Methyloctahydronaphthalen-2(1H)-one		
67	949-41-7	1a,9b-Dihydro-1H-cyclopropa[1]phenanthrene		
67	95-47-6	o-Xylene		
67	95-63-6	1,2,4-Trimethylbenzene		
67	959103-74-3	Undecyl heptafluorobutanoate		
67	95-93-2	1,2,4,5-Tetramethylbenzene		
67	99-87-6	p-Cymene		
68	16984-48-8	Fluoride	1100	mg/L
68	7429-90-5	Aluminum	137	mg/L
68	7439-89-6	Iron	312	mg/L
68	7439-96-5	Manganese	29	mg/L
68	7439-98-7	Molybdenum	3.49	mg/L
68	7440-38-2	Arsenic	3.16	mg/L
68	7440-39-3	Barium	900	mg/L
68	7440-42-8	Boron	90	mg/L
68	7440-47-3	Chromium	83.9	mg/L
68	7440-50-8	Copper	24.2	mg/L
68	7440-66-6	Zinc	26.9	mg/L
68	7782-49-2	Selenium	1.34	mg/L
69	7440-09-7	Potassium	294	mg/L
69	14127-61-8	Calcium ion	9994	mg/L
69	14797-55-8	Nitrate	18.1	mg/L
69	14808-79-8	Sulfate	31.7	mg/L
69	16887-00-6	Chloride	91800	mg/L
69	17341-25-2	Sodium ion	44770	mg/L
69	24959-67-9	Bromide	876	mg/L
69	7439-89-6	Iron	109	mg/L
69	7439-95-4	Magnesium	1255	mg/L
69	7440-24-6	Strontium	2687	mg/L
69	7440-39-3	Barium	3169	mg/L
69	7704-34-9	Sulfur	56.8	mg/L
70	7440-09-7	Potassium	261	mg/L
70	14808-79-8	Sulfate	25.7	mg/L
70	16887-00-6	Chloride	51000	mg/L
70	17341-25-2	Sodium ion	20910	mg/L
70	24959-67-9	Bromide	552	mg/L
70	71-50-1	Acetate	75.9	mg/L
70	7439-89-6	Iron	64.9	mg/L
70	7440-24-6	Strontium	1296	mg/L
70	7440-39-3	Barium	418	mg/L
70	7440-70-2	Calcium	8818	mg/L
70	7553-56-2	Iodine	10.3	mg/L
71	7440-09-7	Potassium	53	mg/L
71	14797-55-8	Nitrate	7	mg/L
71	14808-79-8	Sulfate	60	mg/L
71	16887-00-6	Chloride	3361	mg/L
71	71-52-3	Bicarbonate	528	mg/L
71	7439-89-6	Iron	0.39	mg/L
71	7439-95-4	Magnesium	9.1	mg/L
71	7439-96-5	Manganese	0.26	mg/L
71	7440-23-5	Sodium	2252	mg/L
71	7440-42-8	Boron	28	mg/L
71	7440-70-2	Calcium	56	mg/L
72	13233-32-4	Radium-224	567.5675676	pCi/L
72	13966-00-2	Potassium-40	270.2702703	pCi/L
72	13966-29-5	Uranium 234	0.06972973	pCi/L
72	13981-52-7	Polonium-210	111.6216216	pCi/L
72	14274-82-9	Thorium 228	595.1351351	pCi/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
72	14331-83-0	Actinium-228	2054.054054	pCi/L
72	14733-03-0	Bismuth-214	6351.351351	pCi/L
72	15067-28-4	Lead-214	6918.918919	pCi/L
72	15092-94-1	Lead-212	64.86486486	pCi/L
72	15117-96-1	Uranium-235	0.003783784	pCi/L
72	7440-61-1	Uranium	0.030540541	pCi/L
73	7440-09-7	Potassium	160	mg/L
73	13982-63-3	Radium-226	16486.48649	pCi/L
73	14265-44-2	Phosphate	8	mg/L
73	16887-00-6	Chloride	147000	mg/L
73	24959-67-9	Bromide	1300	mg/L
73	471-34-1	Carbonic acid calcium salt (1:1)	10	mg/L
73	68334-30-5	Fuels, diesel	1.3	mg/L
73	7439-89-6	Iron	43	mg/L
73	7439-92-1	Lead	1	mg/L
73	7439-95-4	Magnesium	850	mg/L
73	7439-96-5	Manganese	3.4	mg/L
73	7440-21-3	Silicon	3.7	mg/L
73	7440-23-5	Sodium	29000	mg/L
73	7440-24-6	Strontium	36000	mg/L
73	7440-38-2	Arsenic	0.81	mg/L
73	7440-39-3	Barium	9000	mg/L
73	7440-70-2	Calcium	13000	mg/L
73	8008-20-6	Kerosine	0.2	mg/L
73	86290-81-5	Gasoline	0.8	mg/L
74	7440-09-7	Potassium		
74	100-41-4	Ethylbenzene		
74	10045-97-3	Caesium-137		
74	100-51-6	Benzyl alcohol		
74	1024-57-3	Heptachlor epoxide		
74	105-67-9	2,4-Dimethylphenol		
74	106-44-5	p-Cresol		
74	107-13-1	Acrylonitrile		
74	107-21-1	Ethylene glycol		
74	108-39-4	m-Cresol		
74	108-67-8	1,3,5-Trimethylbenzene		
74	108-88-3	Toluene		
74	108-95-2	Phenol		
74	109-06-8	2-Methylpyridine		
74	110-86-1	Pyridine		
74	111-44-4	Bis(2-chloroethyl) ether		
74	117-81-7	Di(2-ethylhexyl) phthalate		
74	122-39-4	Diphenylamine		
74	124-38-9	Carbon dioxide		
74	124-48-1	Chlorodibromomethane		
74	12672-29-6	Aroclor 1248		
74	127-18-4	Tetrachloroethylene		
74	1330-20-7	Xylenes		
74	13982-63-3	Radium-226		
74	14265-45-3	Sulfite		
74	14797-55-8	Nitrate		
74	14797-65-0	Nitrite		
74	14808-79-8	Sulfate		
74	15262-20-1	Radium-228		
74	16065-83-1	Chromium (III)		
74	16887-00-6	Chloride		
74	16984-48-8	Fluoride		
74	18540-29-9	Chromium (VI) ion		
74	191-24-2	Benzo(g,h,i)perylene		
74	193-39-5	Indeno(1,2,3-cd)pyrene		
74	205-99-2	Benzo(b)fluoranthene		
74	206-44-0	Fluoranthene		
74	207-08-9	Benzo(k)fluoranthene		
74	24959-67-9	Bromide		
74	309-00-2	Aldrin		
74	319-85-7	beta-Hexachlorocyclohexane		
74	33213-65-9	Endosulfan II		
74	50-32-8	Benzo(a)pyrene		
74	53-70-3	Dibenz(a,h)anthracene		
74	57-12-5	Cyanide		
74	57-55-6	1,2-Propylene glycol		
74	57-97-6	7,12-Dimethylbenz(a)anthracene		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
74	58-89-9	Lindane		
74	64-19-7	Acetic acid		
74	67-56-1	Methanol		
74	67-63-0	Isopropanol		
74	67-64-1	Acetone		
74	67-66-3	Chloroform		
74	71-43-2	Benzene		
74	72-55-9	p,p'-DDE		
74	7421-93-4	Endrin aldehyde		
74	7429-90-5	Aluminum		
74	7439-89-6	Iron		
74	7439-92-1	Lead		
74	7439-93-2	Lithium		
74	7439-95-4	Magnesium		
74	7439-96-5	Manganese		
74	7439-97-6	Mercury		
74	7439-98-7	Molybdenum		
74	7440-02-0	Nickel		
74	7440-14-4	Radium		
74	7440-22-4	Silver		
74	7440-23-5	Sodium		
74	7440-24-6	Strontium		
74	7440-28-0	Thallium		
74	7440-32-6	Titanium		
74	7440-36-0	Antimony		
74	7440-38-2	Arsenic		
74	7440-39-3	Barium		
74	7440-41-7	Beryllium		
74	7440-42-8	Boron		
74	7440-43-9	Cadmium		
74	7440-47-3	Chromium		
74	7440-48-4	Cobalt		
74	7440-50-8	Copper		
74	7440-62-2	Vanadium		
74	7440-66-6	Zinc		
74	7440-67-7	Zirconium		
74	7440-70-2	Calcium		
74	74-83-9	Methyl bromide		
74	74-87-3	Chloromethane		
74	75-15-0	Carbon disulfide		
74	75-25-2	Bromoform		
74	75-27-4	Bromodichloromethane		
74	76-44-8	Heptachlor		
74	7664-41-7	Ammonia		
74	7723-14-0	Phosphorus		
74	7782-49-2	Selenium		
74	78-93-3	Methyl ethyl ketone		
74	84-74-2	Dibutyl phthalate		
74	85-01-8	Phenanthrene		
74	86-30-6	N-Nitrosodiphenylamine		
74	86-73-7	Fluorene		
74	87-61-6	1,2,3-Trichlorobenzene		
74	87-65-0	2,6-Dichlorophenol		
74	91-20-3	Naphthalene		
74	91-57-6	2-Methylnaphthalene		
74	94-59-7	Safrole		
74	95-48-7	o-Cresol		
74	95-63-6	1,2,4-Trimethylbenzene		
74	959-98-8	Endosulfan I		
74	98-82-8	Cumene		
74	98-86-2	Acetophenone		
75	7440-09-7	Potassium	430	mg/L
75	14127-61-8	Calcium ion		
75	14808-79-8	Sulfate		
75	15438-31-0	Fe +2 ion	22	mg/L
75	16887-00-6	Chloride		
75	17341-25-2	Sodium ion		
75	24959-67-9	Bromide		
75	25322-68-3	Polyethylene glycol	16	mg/L
75	68213-23-0	Alcohols, C12-18, ethoxylated	0.3	mg/L
75	7439-95-4	Magnesium		
75	7553-56-2	Iodine	40.8	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
75	8001-54-5	Benzalkonium chloride		1 mg/L
76	10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one		
76	105-60-2	Caprolactam		
76	107-21-1	Ethylene glycol		
76	107997-59-1	1,2,3-Trimethyl-4-(3-methylbutyl)benzene		
76	112-34-5	2-(2-Butoxyethoxy)ethanol		
76	115-86-6	Triphenyl phosphate		
76	117-81-7	Di(2-ethylhexyl) phthalate		
76	117-84-0	Di-n-octyl phthalate		
76	119-61-9	Benzophenone		
76	119-64-2	Tetralin		
76	119-65-3	Isoquinoline		
76	122-39-4	Diphenylamine		
76	129-00-0	Pyrene		
76	1300-71-6	Dimethylphenol		
76	1321-94-4	Methylnaphthalene		
76	132-65-0	Dibenzothiophene		
76	134-62-3	DEET		
76	140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol		
76	143-07-7	Dodecanoic acid		
76	144-19-4	2,2,4-Trimethyl-1,3-pentanediol		
76	1483-60-9	2,4-Dimethyl-1-(1-methylpropyl)benzene		
76	198-55-0	Perylene		
76	2315-61-9	2-[2-[4-(1,1,3,3-Tetramethylbutyl)phenoxy]ethoxy]ethanol		
76	243-38-9	5H-Quinindoline		
76	25167-82-2	Trichlorophenol		
76	25551-13-7	Trimethylbenzene		
76	26603-23-6	Bis(octylphenyl)amine		
76	26746-38-3	2,3-di-tert-butylphenol		
76	272-16-2	1,2-Benzisothiazole		
76	28652-72-4	Methyl-1,1'-biphenyl		
76	28804-88-8	Dimethylnaphthalene		
76	3055-93-4	2-[2-(Dodecyloxy)ethoxy]ethanol		
76	3055-94-5	Triethylene glycol monododecyl ether		
76	3333-52-6	Tetramethylsuccinonitrile		
76	4013-34-7	(1-Methoxyethyl)benzene		
76	4466-77-7	1,2,3,4-Tetramethylphenanthrene		
76	483-65-8	Retene		
76	544-63-8	Tetradecanoic acid		
76	54827-17-7	3,3',5,5'-Tetramethylbenzidine		
76	562-28-7	(-)-Kaur-16-ene		
76	57-10-3	Hexadecanoic acid		
76	57-11-4	Octadecanoic acid		
76	629-62-9	Pentadecane		
76	629-99-2	Pentacosane		
76	6971-52-4	3-Methoxy-2-methylphenol		
76	80-05-7	Bisphenol A		
76	80061-31-0	3,4-Dihydro-1,9(2H,10H)-acridinedione		
76	84-66-2	Diethyl phthalate		
76	84-74-2	Dibutyl phthalate		
76	84-77-5	Didecyl phthalate		
76	85-68-7	Benzyl butyl phthalate		
76	874-41-9	1,3-Dimethyl-4-ethylbenzene		
76	88-18-6	2-tert-Butylphenol		
76	90-12-0	1-Methylnaphthalene		
76	91-20-3	Naphthalene		
76	91-22-5	Quinoline		
76	91-57-6	2-Methylnaphthalene		
76	92-52-4	Biphenyl		
76	934-34-9	Benzothiazolone		
76	95-16-9	Benzothiazole		
76	96-76-4	2,4-Di-tert-butylphenol		
76	98-54-4	4-tert-Butylphenol		
76	98-86-2	Acetophenone		
76	NOCAS_891518	Nonylphenols		
77	1002-84-2	Pentadecanoic acid	0.00084	mg/L
77	100-51-6	Benzyl alcohol	0.00033	mg/L
77	1016165-79-9	1,2-Di-but-2-enyl-cyclohexane	0.00077	mg/L
77	101-81-5	Diphenylmethane	0.00043	mg/L
77	106-51-4	1,4-Benzoquinone	0.00008	mg/L
77	1079-71-6	1,2,3,4,5,6,7,8-Octahydroanthracene	0.00054	mg/L
77	108837-05-4	4-Propyl-9H-xanthen-9-one	0.00007	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
77	109-21-7	Butyl butyrate	0.00044	mg/L
77	110-27-0	Isopropyl tetradecanoic acid	0.00179	mg/L
77	112-34-5	2-(2-Butoxyethoxy)ethanol	0.00045	mg/L
77	115-86-6	Triphenyl phosphate	0.00021	mg/L
77	117-84-0	Di-n-octyl phthalate	0.00463	mg/L
77	119296-91-2	Methyl (4Z)-3,3-diphenylhex-4-enoate	0.002	mg/L
77	119-64-2	Tetralin	0.00082	mg/L
77	1203-17-4	2,3-Dihydro-1,1,2,3,3-pentamethyl-1H-indene	0.00045	mg/L
77	1205-39-6	2-Methyl-N-phenylaniline	0.00353	mg/L
77	121-33-5	4-Hydroxy-3-methoxybenzaldehyde	0.00431	mg/L
77	122-39-4	Diphenylamine	0.00373	mg/L
77	123731-75-9	1-Allyl-3-methylindole-2-carbaldehyde	0.00149	mg/L
77	1241-94-7	2-Ethylhexyl diphenyl phosphate	0.00075	mg/L
77	126-73-8	Tributyl phosphate	0.01896	mg/L
77	129-00-0	Pyrene	0.00004	mg/L
77	1300-71-6	Dimethylphenol	0.00138	mg/L
77	131-11-3	Dimethyl phthalate	0.00028	mg/L
77	1321-94-4	Methylnaphthalene	0.00048	mg/L
77	136-83-4	2-Nonylphenol	0.00791	mg/L
77	143-07-7	Dodecanoic acid	0.0017	mg/L
77	1450-72-2	1-(2-Hydroxy-5-methylphenyl)ethanone	0.00029	mg/L
77	149-30-4	2-Mercaptobenzothiazole	0.00089	mg/L
77	15123-40-7	Pyreno[4,5-c]furan	0.00183	mg/L
77	1559-81-5	1-Methyltetraline	0.00069	mg/L
77	1599-67-3	1-Docosene	0.00233	mg/L
77	160951-15-5	4,6,8-Trimethyl-2-propylazulene	0.0004	mg/L
77	1620-98-0	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	0.00042	mg/L
77	1689-64-1	Fluoren-9-ol	0.00032	mg/L
77	1730-37-6	1-Methylfluorene	0.00051	mg/L
77	18435-45-5	1-Nonadecene	0.00215	mg/L
77	18835-33-1	1-Hexacosene	0.00204	mg/L
77	19781-86-3	8-Hexadecyne	0.00028	mg/L
77	20291-73-0	Dimethylphenanthrene	0.00149	mg/L
77	204781-73-7	28-Nor-17alpha(H)-hopane	0.00126	mg/L
77	2103-57-3	2,3,4-Trimethoxybenzaldehyde	0.00039	mg/L
77	228729-94-0	8,13-Dimethyl-14-(3-methylbutyl)podocarpene	0.00175	mg/L
77	2315-61-9	2-[2-[4-(1,1,3,3-Tetramethylbutyl)phenoxy]ethoxy]ethanol	0.00134	mg/L
77	2381-21-7	1-Methylpyrene	0.00002	mg/L
77	2440-22-4	2-(2H-Benzotriazol-2-yl)-4-methylphenol	0.00091	mg/L
77	24624-29-1	1-Ethyl-9,10-anthraquinone	0.00012	mg/L
77	25167-94-6	Diphenylpropane	0.00022	mg/L
77	25377-73-5	3-(Dodecenyldihydro-2,5-furandione	0.00116	mg/L
77	26603-23-6	Bis(octylphenyl)amine	0.00019	mg/L
77	27519-02-4	(Z)-9-Tricosene	0.00098	mg/L
77	27530-79-6	Simonellite	0.00068	mg/L
77	276890-11-0	5-(1,1-Dimethylethyl)-1H-indene	0.0001	mg/L
77	27875-89-4	1-Phenanthrenecarboxylic acid	0.00012	mg/L
77	28652-72-4	Methyl-1,1'-biphenyl	0.001	mg/L
77	28804-88-8	Dimethylnaphthalene	0.00144	mg/L
77	28981-49-9	Ethylcyclododecane	0.00154	mg/L
77	297-35-8	Cyclotriacontane	0.00108	mg/L
77	30232-26-9	Trimethylphenanthrene	0.00012	mg/L
77	309735-29-3	1,2-Benzisothiazole, 3-(hexahydro-1H-azepin-1-yl)-, 1,1-dioxide	0.00066	mg/L
77	3386-33-2	Octadecyl chloride	0.00212	mg/L
77	35216-11-6	7-Tetradecyne	0.00038	mg/L
77	3891-98-3	2,6,10-Trimethyldodecane	0.00096	mg/L
77	4466-77-7	1,2,3,4-Tetramethylphenanthrene	0.00068	mg/L
77	48134-26-5	2,4,6-Trimethylazulene	0.00049	mg/L
77	483-65-8	Retene	0.00319	mg/L
77	483-78-3	Cadalene	0.00032	mg/L
77	4957-14-6	1-Methyl-4-[(4-methylphenyl)methyl]benzene	0.00011	mg/L
77	50-24-8	Prednisolone	0.00051	mg/L
77	52845-07-5	Isoeicosane	0.00258	mg/L
77	5337-61-1	2-Octadecyl-1,3-propanediol	0.00042	mg/L
77	544-63-8	Tetradecanoic acid	0.00054	mg/L
77	5466-77-3	Octinoxate	0.00278	mg/L
77	55045-07-3	2-Methyl-8-propyldodecane	0.00052	mg/L
77	562-28-7	(-)-Kaur-16-ene	0.00136	mg/L
77	57-10-3	Hexadecanoic acid	0.00256	mg/L
77	57-88-5	Cholesterol	0.00026	mg/L
77	58-08-2	Caffeine	0.0005	mg/L
77	593-49-7	Heptacosane	0.00095	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
77	599-64-4	4-Cumylphenol	0.00118	mg/L
77	610-48-0	1-Methylantracene	0.00048	mg/L
77	615-22-5	2-(Methylthio)benzothiazole	0.00054	mg/L
77	61819-81-6	2,3',5-Trimethyldiphenylmethane	0.00005	mg/L
77	62583-58-8	1-Butyl-2-ethyloctahydro-1H-4,7-epoxyinden-5-ol	0.0009	mg/L
77	629-59-4	Tetradecane	0.00054	mg/L
77	629-97-0	Docosane	0.00194	mg/L
77	629-99-2	Pentacosane	0.00154	mg/L
77	630-01-3	Hexacosane	0.00173	mg/L
77	63521-76-6	Tridecanedial	0.00086	mg/L
77	638-36-8	2,6,10,14-Tetramethylhexadecane	0.00165	mg/L
77	638-67-5	Tricosane	0.0017	mg/L
77	646-31-1	Tetracosane	0.00186	mg/L
77	65119-95-1	22-Tricosenoic acid	0.00043	mg/L
77	68593-94-2	2-Ethenylphenanthrene	0.00022	mg/L
77	6971-40-0	17-pentatriacontene	0.001	mg/L
77	719-22-2	2,6-Bis-(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione	0.00028	mg/L
77	73493-71-7	9-Methoxy-9H-fluorene	0.00018	mg/L
77	74646-38-1	4,4-Dimethyltetracyclo[5.2.1.02,6.03,5]decane	0.00027	mg/L
77	7683-64-9	Squalene	0.00024	mg/L
77	790-82-9	4,4'-Diacetyldiphenylmethane	0.00037	mg/L
77	80-05-7	Bisphenol A	0.01617	mg/L
77	80061-31-0	3,4-Dihydro-1,9(2H,10H)-acridinedione	0.00135	mg/L
77	830-09-1	4-Methoxycinnamic acid	0.00016	mg/L
77	84-66-2	Diethyl phthalate	0.0149	mg/L
77	84-74-2	Dibutyl phthalate	0.00127	mg/L
77	84-77-5	Didecyl phthalate	0.00723	mg/L
77	85-01-8	Phenanthrene	0.00052	mg/L
77	85-68-7	Benzyl butyl phthalate	0.00033	mg/L
77	86-73-7	Fluorene	0.00024	mg/L
77	879-12-9	1,2,3-Trimethylnaphthalene	0.0026	mg/L
77	91-20-3	Naphthalene	0.00066	mg/L
77	92513-28-5	3-Methylquinoline-2-carboxylic acid	0.00665	mg/L
77	92-52-4	Biphenyl	0.0003	mg/L
77	934-34-9	Benzothiazolone	0.0039	mg/L
77	93927-20-9	1-Ethyl-2-methylnaphthalene	0.00055	mg/L
77	941228-34-8	7-(Bromomethyl)pentadec-7-ene	0.00277	mg/L
77	95-16-9	Benzothiazole	0.01427	mg/L
77	98-54-4	4-tert-Butylphenol	0.00019	mg/L
77	NOCAS_873040	Tricyclo[4.4.0.0(3,9)]decane	0.00026	mg/L
77	NOCAS_873049	Tetrahydrophenanthrene	0.00042	mg/L
77	NOCAS_873051	Ethyltetrahydronaphthalene	0.00046	mg/L
78	14127-61-8	Calcium ion	7890	mg/L
78	16887-00-6	Chloride	127249	mg/L
78	17341-25-2	Sodium ion	63686	mg/L
78	71-52-3	Bicarbonate	228	mg/L
79	12587-46-1	Alpha particle		
79	12587-47-2	Beta particle		
79	13982-63-3	Radium-226		
79	15262-20-1	Radium-228		
80	7440-09-7	Potassium	1784	mg/L
80	7429-90-5	Aluminum	11.32	mg/L
80	7439-89-6	Iron	248.6	mg/L
80	7439-93-2	Lithium	168.4	mg/L
80	7439-95-4	Magnesium	2058	mg/L
80	7439-96-5	Manganese	12.43	mg/L
80	7440-21-3	Silicon	11.47	mg/L
80	7440-23-5	Sodium	54350	mg/L
80	7440-24-6	Strontium	7442	mg/L
80	7440-39-3	Barium	2927	mg/L
80	7440-42-8	Boron	28.66	mg/L
80	7440-50-8	Copper	1.215	mg/L
80	7440-66-6	Zinc	1.143	mg/L
80	7440-70-2	Calcium	29490	mg/L
80	7704-34-9	Sulfur	43.79	mg/L
80	7723-14-0	Phosphorus	3.521	mg/L
81	14797-55-8	Nitrate	10.05	mg/L
81	14797-65-0	Nitrite	25.5	mg/L
81	16887-00-6	Chloride	51288	mg/L
81	24959-67-9	Bromide	693	mg/L
81	7553-56-2	Iodine	54	mg/L
81	7664-41-7	Ammonia	66.28	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
82	10544-50-0	Octasulfur		
82	105-60-2	Caprolactam		
82	115-86-6	Triphenyl phosphate		
82	117-84-0	Di-n-octyl phthalate		
82	126-73-8	Tributyl phosphate		
82	128-39-2	2,6-Di-tert-butylphenol		
82	140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol		
82	143-07-7	Dodecanoic acid		
82	18496-25-8	Sulfide		
82	27601-00-9	Methylquinoline		
82	28652-72-4	Methyl-1,1'-biphenyl		
82	544-63-8	Tetradecanoic acid		
82	57-10-3	Hexadecanoic acid		
82	57-11-4	Octadecanoic acid		
82	7440-17-7	Rubidium		
82	7440-46-2	Cesium		
82	7553-56-2	Iodine		
82	91-20-3	Naphthalene		
82	95-16-9	Benzothiazole		
83	7440-09-7	Potassium		
83	10544-50-0	Octasulfur	0.009629866	mg/L
83	105-60-2	Caprolactam	0.002392004	mg/L
83	115-86-6	Triphenyl phosphate	0.00677137	mg/L
83	117-81-7	Di(2-ethylhexyl) phthalate	0.002296103	mg/L
83	124-38-9	Carbon dioxide	634	mg/L
83	126-73-8	Tributyl phosphate	0.002664287	mg/L
83	1321-94-4	Methylnaphthalene	0.015553579	mg/L
83	140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol	0.018338478	mg/L
83	14265-44-2	Phosphate	3.57	mg/L
83	143-07-7	Dodecanoic acid	0.002517211	mg/L
83	14797-55-8	Nitrate	27.8	mg/L
83	14797-65-0	Nitrite	0.633	mg/L
83	14808-79-8	Sulfate	302	mg/L
83	16887-00-6	Chloride	42800	mg/L
83	16984-48-8	Fluoride	22.6	mg/L
83	24959-67-9	Bromide	0.15	mg/L
83	25447-95-4	Hexadecenoic acid	0.008368372	mg/L
83	26764-26-1	Octadecenoic acid	0.003472104	mg/L
83	27601-00-9	Methylquinoline	0.003749272	mg/L
83	28652-72-4	Methyl-1,1'-biphenyl	0.00213067	mg/L
83	28804-88-8	Dimethylnaphthalene	0.009506014	mg/L
83	3812-32-6	Carbonate	64	mg/L
83	544-63-8	Tetradecanoic acid	0.005315497	mg/L
83	57-10-3	Hexadecanoic acid	0.003021193	mg/L
83	57-11-4	Octadecanoic acid	0.00373392	mg/L
83	71-52-3	Bicarbonate	978	mg/L
83	7429-90-5	Aluminum	0.099	mg/L
83	7439-89-6	Iron	93.1	mg/L
83	7439-92-1	Lead	0.155	mg/L
83	7439-93-2	Lithium	8.94	mg/L
83	7439-95-4	Magnesium	392	mg/L
83	7439-96-5	Manganese	4.84	mg/L
83	7439-97-6	Mercury	0.000023	mg/L
83	7439-98-7	Molybdenum	0.067	mg/L
83	7440-02-0	Nickel	0.358	mg/L
83	7440-23-5	Sodium	16700	mg/L
83	7440-24-6	Strontium	142	mg/L
83	7440-28-0	Thallium	0.0386	mg/L
83	7440-31-5	Tin	0.0086	mg/L
83	7440-36-0	Antimony	0.0219	mg/L
83	7440-38-2	Arsenic	0.0122	mg/L
83	7440-39-3	Barium	281	mg/L
83	7440-41-7	Beryllium	0.0014	mg/L
83	7440-42-8	Boron	0.493	mg/L
83	7440-43-9	Cadmium	0.012	mg/L
83	7440-48-4	Cobalt	0.115	mg/L
83	7440-62-2	Vanadium	0.0386	mg/L
83	7440-66-6	Zinc	0.278	mg/L
83	7440-70-2	Calcium	1350	mg/L
83	7631-86-9	Silica	18.1	mg/L
83	7664-41-7	Ammonia	8.91	mg/L
83	7723-14-0	Phosphorus	3.25	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
83	7727-37-9	Nitrogen	38.4	mg/L
83	7782-49-2	Selenium	0.0407	mg/L
83	879-12-9	1,2,3-Trimethylnaphthalene	0.004485087	mg/L
83	91-20-3	Naphthalene	0.006566544	mg/L
83	95-16-9	Benzothiazole	0.00304147	mg/L
83	96-76-4	2,4-Di-tert-butylphenol	0.004941527	mg/L
84	7440-09-7	Potassium	2260	mg/L
84	14798-03-9	Ammonium	976	mg/L
84	14808-79-8	Sulfate	3100	mg/L
84	16887-00-6	Chloride	185000	mg/L
84	16984-48-8	Fluoride	7.3	mg/L
84	24959-67-9	Bromide	218	mg/L
84	71-52-3	Bicarbonate	560	mg/L
84	7439-93-2	Lithium	24600	mg/L
84	7439-95-4	Magnesium	859	mg/L
84	7439-96-5	Manganese	931	mg/L
84	7440-23-5	Sodium	104000	mg/L
84	7440-39-3	Barium	4060	mg/L
84	7440-42-8	Boron	176000	mg/L
84	7440-46-2	Cesium	537	mg/L
84	7440-70-2	Calcium	8441	mg/L
85	7440-09-7	Potassium	2040	mg/L
85	14808-79-8	Sulfate	1230	mg/L
85	16887-00-6	Chloride	121000	mg/L
85	16984-48-8	Fluoride	2.65	mg/L
85	24959-67-9	Bromide	240	mg/L
85	471-34-1	Carbonic acid calcium salt (1:1)	142	mg/L
85	7439-93-2	Lithium	31.9	mg/L
85	7439-95-4	Magnesium	961	mg/L
85	7439-96-5	Manganese	0.101	mg/L
85	7440-17-7	Rubidium	4.37	mg/L
85	7440-23-5	Sodium	70500	mg/L
85	7440-24-6	Strontium	16.8	mg/L
85	7440-39-3	Barium	0.856	mg/L
85	7440-42-8	Boron	230	mg/L
85	7440-70-2	Calcium	5030	mg/L
85	7553-56-2	Iodine	29.5	mg/L
86	7440-09-7	Potassium	473	mg/L
86	14808-79-8	Sulfate	4880	mg/L
86	16887-00-6	Chloride	20600	mg/L
86	17341-25-2	Sodium ion	13900	mg/L
86	24959-67-9	Bromide	13.7	mg/L
86	71-52-3	Bicarbonate	1800	mg/L
86	7429-90-5	Aluminum	0.406	mg/L
86	7439-93-2	Lithium	2.36	mg/L
86	7439-95-4	Magnesium	486	mg/L
86	7439-96-5	Manganese	0.648	mg/L
86	7440-02-0	Nickel	0.356	mg/L
86	7440-17-7	Rubidium	0.276	mg/L
86	7440-21-3	Silicon	12.2	mg/L
86	7440-24-6	Strontium	36.8	mg/L
86	7440-39-3	Barium	0.0573	mg/L
86	7440-42-8	Boron	4.64	mg/L
86	7440-50-8	Copper	0.0168	mg/L
86	7440-61-1	Uranium	0.0021	mg/L
86	7440-70-2	Calcium	1600	mg/L
87	7439-96-5	Manganese	11.2	mg/L
87	7440-39-3	Barium	12000	mg/L
87	7440-61-1	Uranium	0.00326	mg/L
88	17341-25-2	Sodium ion	69500	mg/L
88	7439-93-2	Lithium	233	mg/L
89	2157-01-9	Octyl methacrylate		
89	2272-03-9	Butylidencyclohexane		
89	2274-11-5	Ethylene acrylate		
89	2883-05-8	Octane, 2-cyclohexyl-		
89	2884-06-2	2,3-Dimethylnonane		
89	2935-07-1	1H-Phenalene, dodecahydro-		
89	5744-03-6	1H-Fluorene, dodecahydro-		
89	5911-04-6	3-Methylnonane		
89	7440-09-7	Potassium	101.15	mg/L
89	1002-43-3	Undecane, 3-methyl-		
89	1003-64-1	Cyclohexane, ethylidene-		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
89	100463-01-2	2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (cis)		
89	100-49-2	Cyclohexanemethanol		
89	1008-80-6	2,3-Dimethyldecahydronaphthalene		
89	10374-74-0	7-Tetradecene		
89	105882-89-1	Ethanamine, 2,2'-azobis[N,N,1,1,2,2-hexafluoro-		
89	106-90-1	Glycidyl acrylate		
89	111-84-2	Nonane		
89	1120-21-4	Undecane		
89	1123-09-7	2-Cyclohexen-1-one, 3,5-dimethyl-		
89	112-39-0	Methyl hexadecanoate		
89	112-40-3	Dodecane		
89	1124-25-0	Cyclohexane, 1-methyl-4-(1-methylethenyl)-, trans-		
89	112-62-9	Methyl (9Z)-octadec-9-enoate		
89	1137-00-4	d,l-7-Azatryptophan		
89	114482-57-4	4-Cyanophenyl 4-(3-butenyloxy)benzoate		
89	114774-79-7	p-Nitrophenyl 1-azetidinedicarboxylate		
89	116164-06-8	3-Heptene, 2,2,3,5,6-pentamethyl-		
89	118252-04-3	1-Hexyl-2-nitrocyclohexane		
89	1193-79-9	5-Methyl-2-furylmethylketone		
89	122-84-9	2-Propanone, 1-(4-methoxyphenyl)-		
89	13066-95-0	1,3-Benzenediol, 4-amino-		
89	13150-81-7	2,6-Dimethyldecane		
89	13151-34-3	3-Methyldecane		
89	13151-35-4	5-Methyldecane		
89	13151-63-8	Cyclodecene, 1-methyl-, (E)-		
89	13287-21-3	6-Methyltridecane		
89	13472-79-2	2-Hydroxy-5-iodopyridine		
89	13485-66-0	2(1H)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-4a,8a-dimethyl-, cis-		
89	135241-50-8	Propanamide, 2-(4-isobutylphenyl)-N-(3,5-dinitrophenyl)-		
89	13726-52-8	Diethyl N-(4-aminobenzoyl)-L-glutamate		
89	13925-05-8	Pyrazine, 2-methyl-5-(1-methylethyl)-		
89	13943-77-6	Naphthalene, 1,2,3,4,4a,5,6,7-octahydro-4a-methyl-		
89	14127-61-8	Calcium ion	2392.03	mg/L
89	142132-75-0	Propane, 1-(di-t-butylphosphino)-3-(2,4,6-tri-t-butylphenyl)phosphino-		
89	14339-23-2	1H-Pyrazole, 5-ethyl-4,5-dihydro-1,4-dimethyl-		
89	14360-50-0	1-Hexanone, 1-(2-furanyl)-		
89	14449-42-4	1-sec-Butyladamantane		
89	14451-87-7	Tricyclo(3.3.1.13,7)decane, 2-ethyl-		
89	14451-88-8	2-n-Propyladamantane		
89	1454-84-8	n-Nonadecanol-1		
89	14676-29-0	3-Ethyl-2-methylheptane		
89	14808-79-8	Sulfate	41.7	mg/L
89	1486-75-5	cyclododecene, (e)-		
89	1502-38-1	Cyclooctane, methyl-		
89	1522-22-1	1,1,1,5,5,5-Hexafluoroacetylacetone		
89	15232-78-7	Cyclohexene,3-hexyl-		
89	15232-86-7	1-Heptylcyclohexene		
89	1528-22-9	Cyclobutane, (1-methylethylidene)-		
89	15496-01-2	Ditrifluoromethyl(chlorocarbonyloxy)amine		
89	1560-96-9	2-Methyltridecane		
89	1560-97-0	2-Methylododecane		
89	15869-93-9	3,5-Dimethyloctane		
89	1595-16-0	1-(Butan-2-yl)-4-methylbenzene		
89	1606-08-2	Cyclopentylcyclohexane		
89	1618-22-0	naphthalene, decahydro-2,6-dimethyl-		
89	1632-70-8	Undecane, 5-methyl-		
89	1636-44-8	Decane, 4-ethyl-		
89	16538-89-9	cyclooctane, (1-methylpropyl)-		
89	16580-24-8	1-Methyl-3-propan-2-ylcyclohexane		
89	16580-26-0	cyclohexane, 1-isopropyl-1-methyl-		
89	1660-04-4	Methyl tricyclo(3.3.1.13,7)dec-1-yl ketone		
89	1667-00-1	Benzylcyclopropane		
89	166773-56-4	2,3-Dimethyl-5-(2,6,10-trimethylundecyl) furan		
89	16681-68-8	2H-1,2,3-Triazole-4-carbaldehyde		
89	1671-77-8	1-Pentanone, 1-(4-methylphenyl)-		
89	1674-10-8	Cyclohexene, 1,2-dimethyl-		
89	16747-30-1	2,4,4-Trimethylhexane		
89	16747-50-5	Cyclopentane, 1-ethyl-1- methyl-		
89	1678-93-9	Butylcyclohexane		
89	1687-34-9	1-Ethyl-3-methyladamantane		
89	1687-35-0	1,3-Dimethyl-5-ethyladamantane		
89	16887-00-6	Chloride	38414.67	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
89	17301-23-4	2,6-Dimethylundecane		
89	17301-32-5	4,7-Dimethylundecane		
89	17301-94-9	4-Methylnonane		
89	17302-23-7	Nonane, 4,5-dimethyl-		
89	17302-27-1	Nonane, 2,5-dimethyl-		
89	17302-28-2	Nonane, 2,6-dimethyl-		
89	17302-32-8	3,7-Dimethylnonane		
89	17302-33-9	6-Methylundecane		
89	17312-50-4	2,5-Dimethyldecane		
89	17312-53-7	3,6-Dimethyldecane		
89	17312-57-1	3-Methyldodecane		
89	17312-59-3	Undecane, 4-ethyl-		
89	17312-60-6	Undecane, 6-ethyl-		
89	17312-62-8	5-Propyldecane		
89	17312-77-5	2,3-Dimethylundecane		
89	17312-80-0	2,4-Dimethylundecane		
89	17453-94-0	Undecane, 5-ethyl-		
89	1750-51-2	Naphthalene, decahydro-1,6-dimethyl-		
89	176-63-6	Spiro(4-5)decane		
89	17851-53-5	Butyl isobutyl phthalate		
89	1795-15-9	Cyclohexane, octyl-		
89	180-43-8	Spiro(5.5)undecane		
89	18294-04-7	Ethanedioic acid, bis(trimethylsilyl) ester		
89	18344-37-1	heptadecane, 2,6,10,14-tetramethyl-		
89	18435-22-8	Tetradecane, 3-methyl-		
89	1879-07-8	Cyclohexane, 1-methyl-4-(1-methylethenyl)-, cis-		
89	188645-81-0	3,4-Dichlorophenol, tert-butyl(dimethylsilyl) ether		
89	1888-57-9	3-Hexanone, 2,5-dimethyl- (8Cl)(9Cl)		
89	19385-87-6	1,3-Dimethyl-5-n-propyl-adamantane		
89	19549-87-2	2,4-Dimethyl-1-heptene		
89	19550-75-5	2,2-dimethyl-3-heptene trans		
89	19744-64-0	1H-Indene, octahydro-5-methyl-		
89	20278-89-1	Heptane, 3,4,5-trimethyl-		
89	20309-77-7	Cyclopentane, 1,1,3,4-tetramethyl-, trans-		
89	20396-49-0	tert-Butyl cyclohexanecarboxyperoxyate		
89	2049-95-8	tert-Pentylbenzene		
89	2051-30-1	2,6-Dimethyloctane		
89	20633-03-8	2,2,5-Trimethylhexane-3,4-dione		
89	21868-43-9	s-Triazine, 2-amino-4-(piperidinomethyl)-4-piperidino-		
89	219783-06-9	1-Isopropyl-1,4,5-trimethylcyclohexane		
89	22052-84-2	Heptafluoroisopropyl methyl ether		
89	227327-87-9	N-Adamantan-1-ylmethyl-2-chloro-5-nitro-benzamide		
89	2294-72-6	5-Undecyne		
89	23183-11-1	1,1'-Bicycloheptyl		
89	23609-46-3	cyclooctane, 1,2-diethyl-		
89	2437-56-1	1-Tridecene		
89	24451-17-0	ethyl 2-(3,4-dimethylanilino)-2-oxoacetate		
89	24959-67-9	Bromide	325.21	mg/L
89	2499-95-8	Hexyl acrylate		
89	25117-24-2	4-Methyltetradecane		
89	25117-31-1	5-Methyltridecane		
89	25117-32-2	5-Methyltetradecane		
89	25201-40-5	1,6-Heptadien-4-ol, 4-methyl-		
89	2541-75-5	8-heptadecanol		
89	2547-26-4	4a-Methyldecalin		
89	2566-97-4	9,12-octadecadienoic acid, methyl ester, (e,e)-		
89	25711-30-2	1H-Pyrazole-4-carboxaldehyde, 1,5-dimethyl-		
89	26321-98-2	Cyclohexane, (1-ethylpropyl)-		
89	26730-12-1	4-Methyltridecane		
89	26730-14-3	7-Methyltridecane		
89	268543-19-7	1-Ethanone, 1-(1-adamantyl)-2-phenyl-		
89	26967-64-6	Cyclohexane, (1-methylpropyl)-		
89	274691-67-7	Dithiocarbaminic acid, N-cyano-, S-[3-(4-ethylphenyl)-3-oxo-1-propenyl]-S'-methyl diester		
89	2809-64-5	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-		
89	281-23-2	Adamantane		
89	2847-72-5	4-Methyldecane		
89	286-63-5	9-Thiabicyclo[6.1.0]nonane		
89	2882-98-6	n-Nonylcyclopentane		
89	2896-60-8	4-Ethylresorcinol		
89	29053-04-1	Cyclopentane, 1-methyl-3-(2-methylpropyl)-		
89	294-62-2	Cyclododecane		
89	2958-76-1	Decahydro-2-methylnaphthalene		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
89	296-56-0	Cycloeicosane		
89	2980-69-0	4-Methylundecane		
89	30159-17-2	Tricyclo[7.3.0.0(2,6)]dodecane, trans-anti-trans-		
89	30677-34-0	Cyclohexane, ethylmethyl-		
89	3073-66-3	1,1,3-Trimethylcyclohexane		
89	307-55-1	Perfluorododecanoic acid		
89	31061-61-7	Tricyclo[4.3.1.1(3,8)]undecane-3-carboxylic acid, methyl ester		
89	315244-85-0	Pyrazolo[3,4-b]pyran-5-carbonitrile, 1,4-dihydro-6-amino-4-(3,4-dichlorophenyl)-3-methyl-		
89	3178-23-2	Dicyclohexylmethane		
89	32038-83-8	2-Propynenitrile, 3-fluoro-		
89	3282-53-9	Cyclohexene, 1-butyl-		
89	331835-05-3	1-(2,4-Dihydroxybenzoyl)-3-ethyl-5-trifluoromethyl-5-hydroxy-2-pyrazoline		
89	337503-48-7	4-Pentenoic acid, 2,2-diethyl-3-oxo-5-phenyl-, ethyl ester		
89	33933-74-3	3-Heptene, 4-ethyl-		
89	3404-73-7	1-Pentene, 3,3-dimethyl-		
89	3430-33-9	2,6-Dimethyl-3-pyridylamine		
89	343270-50-8	2-(Butyliden-2-one)tetrahydrofuran		
89	34694-70-7	1,3,5,6-Tetramethyladamantane		
89	35216-11-6	7-Tetradecyne		
89	352-70-5	m-Fluorotoluene		
89	35354-38-2	7-Octadecyne, 2-methyl-		
89	36947-68-9	1H-Imidazole, 2-(1-methylethyl)-		
89	371-40-4	4-Fluoroaniline		
89	376-77-2	Decafluorocyclopentane		
89	3777-70-6	2-Hexylfuran		
89	3777-71-7	Furan, 2-heptyl-		
89	38489-80-4	Benzaldehyde, 3-methoxy-, oxime		
89	3891-98-3	2,6,10-Trimethyldodecane		
89	39178-69-3	3-butylcyclohexanone		
89	39546-79-7	Pentylidenecyclohexane		
89	4237-46-1	Benzoyldiphenylmethanol		
89	4282-44-4	Undecane, 1-iodo-		
89	4291-79-6	1-Methyl-2-propyl-cyclohexane		
89	4292-75-5	Hexylcyclohexane		
89	4292-92-6	Pentylcyclohexane		
89	432-04-2	Phosphine, tris(trifluoromethyl)-		
89	4360-57-0	2-Pentadecyl-1,3-dioxolane		
89	4431-89-4	(Cyclopentylmethyl)cyclohexane		
89	4516-69-2	1,1,3-Trimethylcyclopentane		
89	4551-51-3	1H-Indene, octahydro-, cis-		
89	4674-23-1	1,2-Di(2,4,6-trimethylphenyl)ethane		
89	47145-46-0	3,4-Dihydroisoquinolin-7-ol, 1-[4-hydroxybenzyl]-6-methoxy-		
89	489-20-3	1-Isopropyl-2,3-dimethylcyclopentane		
89	497-32-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-5-methylene-		
89	5004-45-5	4-Phenylphthalazin-1(2H)-one		
89	50617-19-1	2,5,8-Triphenyl benzotriazole		
89	50876-32-9	CYCLOHEXANE, 1,1,3,5-TETRAMETHYL-, CIS-		
89	50991-08-7	1,1'-Bicyclohexyl, 2-methyl-, cis-		
89	50991-09-8	1,1'-Bicyclohexyl, 2-methyl-, trans-		
89	526-73-8	1,2,3-Trimethylbenzene		
89	527-54-8	3,4,5-Trimethylphenol		
89	52856-01-6	2-Ethoxy-4,4,5,5-tetramethyloxazoline		
89	52873-50-4	1,3-Dimethyl-5-n-hexyladamantane		
89	52896-87-4	Heptane, 4-(1-methylethyl)-		
89	53366-55-5	Pentylidenecyclopentane		
89	5380-87-0	Furfuryl glycidyl ether		
89	53907-60-1	Cyclopentane, 1,1,3,4-tetramethyl-, cis-		
89	54163-69-8	Isopilocarpine		
89	542-28-9	Tetrahydro-2H-pyran-2-one		
89	54410-98-9	1-nonene, 4,6,8-trimethyl-		
89	54411-17-5	Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1à,2à,4à)-		
89	544-76-3	Hexadecane		
89	54676-39-0	2-BUTYL-1,1,3-TRIMETHYL-CYCLOHEXANE		
89	54699-35-3	1,2,4-Benzenetricarboxylic acid, 1,2-dimethyl ester		
89	54823-95-9	Cyclohexane, 1-(cyclohexylmethyl)-3-methyl-, trans-		
89	54823-98-2	Cyclohexane, 1-(cyclohexylmethyl)-4-methyl-, trans-		
89	54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-		
89	54833-48-6	Heptadecane, 2,6,10,15-tetramethyl		
89	55044-33-2	1h-indene, 2-butyl-5-hexyloctahydro-		
89	55170-90-6	Bicyclo[2.2.1]heptane, 2-(1-buten-3-yl)-		
89	55282-34-3	Cyclohexane, 1,3,5-trimethyl-2-octadecyl-		
89	55402-13-6	2,2,7-Trimethyl-3-octyne		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
89	554-59-6	Carane		
89	557-35-7	octane, 2-bromo-		
89	56292-65-0	2,5-Dimethyldodecane		
89	56292-69-4	Tetradecane, 2,5-dimethyl-		
89	563-16-6	3,3-Dimethylhexane		
89	56325-56-5	Cyclodecene, 3-bromo-		
89	56442-17-2	4-(4-Fluorobenzyloxy)benzaldehyde		
89	5661-80-3	Bicyclo[5.3.0]decane		
89	56936-67-5	Glycine, N-trifluoroacetyl-, isopropyl ester		
89	58422-90-5	1,3-Dioxolane-2-heptanenitrile, à-methyl-è-oxo-2-phenyl-		
89	58462-32-1	trans, trans-3-Ethylbicyclo[4.4.0]decane		
89	588-16-9	3-Methoxyacetanilide		
89	59303-13-8	2-Methyl-5-propionylthiophene		
89	594-91-2	Perfluoro-2-methylbutane		
89	60186-80-3	5-Tridecyne		
89	60212-33-1	4-Tetradecyne		
89	6044-71-9	Dodecane, 6-methyl-		
89	6069-98-3	Cyclohexane, 1-methyl-4-(1-methylethyl)-, cis-		
89	61141-80-8	Cyclohexane, 1,2-diethyl-3-methyl-		
89	61142-24-3	cyclohexane, 1,2,4,5-tetraethyl-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.)-		
89	61142-32-3	Cyclopentene, 1,3-dimethyl-2-(1-methylethyl)-		
89	61142-66-3	cyclopentene, 5-hexyl-3,3-dimethyl-		
89	61142-68-5	1-Hexyl-3-methylcyclopentane		
89	61142-70-9	2,4-Diethyl-1-methylcyclohexane		
89	61177-16-0	Bicyclo[2.2.1]heptane, 2-butyl-		
89	6117-97-1	4-Methyldodecane		
89	61208-94-4	Cyclohexane, (1-methylbutyl)-		
89	615-43-0	o-Iodoaniline		
89	61985-25-9	4-Acetylimidazole		
89	62016-37-9	2,4,6-Trimethyloctane		
89	62108-25-2	Decane, 2,6,7-trimethyl-		
89	62108-27-4	decane, 2,4,6-trimethyl-		
89	621-42-1	3-Acetamidophenol		
89	62185-55-1	Nonane, 4-methyl-5-propyl-		
89	62187-13-7	3-Octene, 2,2-dimethyl-, (E)-		
89	62199-52-4	1,2-Dibutylcyclopentane		
89	62238-11-3	2,3,5-Trimethyl-decane		
89	62238-13-5	2,3,7-Trimethyldecane		
89	62238-15-7	Decane, 2,3,4-trimethyl-		
89	62238-32-8	cyclohexane, 1-ethyl-1,4-dimethyl-, trans-		
89	62376-17-4	1,2-Dimethyl-3-pentyl-4-propylcyclohexane		
89	624-29-3	Cyclohexane, 1,4-dimethyl-, cis-		
89	6248-88-0	Bicyclo[2.2.1]heptane, 1,3,3-trimethyl-		
89	626-03-9	2,4-Dihydroxypyridine		
89	629-50-5	Tridecane		
89	629-59-4	Tetradecane		
89	62960-77-4	4-Octene, 2,6-dimethyl-, [S-(Z)]-		
89	629-73-2	1-Hexadecene		
89	629-78-7	Heptadecane		
89	6305-52-8	2-n-Butyldecahydronaphthalene		
89	63088-19-7	(4R*,5R*,9S*)-5,9-Dimethylspiro[3.5]nonan-1-one		
89	63263-09-2	1,3-Dimethyladamantan-5-carboxylic acid, ethyl ester		
89	63798-30-1	2-Butynamide, N-methyl-		
89	63830-68-2	4-Nonene, 2,3,3-trimethyl-, (Z)-		
89	6418-41-3	tridecane, 3-methyl-		
89	64341-49-7	1-Bromo-3-butene-2-ol		
89	645-10-3	1,7-dimethyl-4-(1-methylethyl)cyclodecane		
89	65996-50-1	1H-Pyrrolo[3,2-d]pyrimidine-2,4(3H,5H)-dione		
89	66552-62-3	Naphthalene, decahydro-1,5-dimethyl-		
89	66660-37-5	Trans, trans-2-ethylbicyclo[4.4.0]decane		
89	66660-38-6	cis, trans-2-Ethylbicyclo[4.4.0]decane		
89	66660-42-2	cis, cis-3-ethylbicyclo[4.4.0]decane		
89	6708-17-4	Bicyclooctyl		
89	6783-92-2	cyclohexane, 1,1,2,3-tetramethyl-		
89	693-13-0	Diisopropylcarbodiimide		
89	69462-10-8	2,2,4-Trimethylpentanenitrile		
89	696-29-7	Cyclohexane, (1-methylethyl)-		
89	6975-98-0	2-Methyldecane		
89	697-82-5	2,3,5-Trimethylphenol		
89	69855-48-7	1-Methyl-4-(methylsulfonyl)bicyclo[2.2.2]octane		
89	702-79-4	1,3-Dimethyladamantane		
89	7040-53-1	Dicyclohexyl methylphosphonate		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
89	7045-70-7	1,3-Diisopropyl cyclohexane		
89	7045-71-8	2-Methylundecane		
89	707-35-7	1,3,5-Trimethyladamantane		
89	7145-99-5	1,3-Benzodioxole, 5-methyl-		
89	71940-29-9	3,4-Dimethyl-2-(3-methyl-butyl)-benzoic acid, methyl ester		
89	7216-42-4	Isonicotinaldehyde 1-oxide		
89	74054-92-5	1,1,6,6-tetramethylspiro[4.4]nonane		
89	7411-16-7	3-Ethyl-1,2,4(1H)-triazole		
89	7439-89-6	Iron	73.31	mg/L
89	7439-95-4	Magnesium	336.28	mg/L
89	7440-23-5	Sodium	17421.58	mg/L
89	7440-24-6	Strontium	1013.25	mg/L
89	7440-39-3	Barium	3350.5	mg/L
89	74421-09-3	cyclopentane, 1,1,3-trimethyl-3-(2-methyl-2-propenyl)-		
89	74630-16-3	Phosphonous dichloride, (1,7,7-trimethylbicyclo[2.2.1]hept-2-yl)-		
89	74663-66-4	Cyclohexane, 1,5-diethyl-2,3-dimethyl-		
89	74663-71-1	cyclohexane, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-		
89	74685-30-6	5-eicosene, (e)-		
89	74685-33-9	3-eicosene, (e)-		
89	74810-41-6	cyclohexane, (2-ethyl-1-methylbutylidene)-		
89	74810-42-7	cyclohexane, (2-ethyl-1-methyl-1-butenyl)-		
89	7524-63-2	2,6-DIMETHYLTETRALINE		
89	754-43-8	2-Bromo-1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)propane		
89	762-42-5	2-Butyenedioic acid, dimethyl ester		
89	78-67-1	Azobisisobutyronitrile		
89	78-77-3	1-Bromo-2-methylpropane		
89	79-03-8	Propanoyl chloride		
89	80655-44-3	Decahydro-4,4,8,9,10-pentamethylnaphthalene		
89	82253-11-0	7-octylidenebicyclo[4.1.0]heptane		
89	823-17-6	Cyclohexene, 3,5-dimethyl-		
89	824-43-1	(1R,2S)-1,2-Diethylcyclohexane		
89	825-44-5	Benzo(b)thiophene 1,1-dioxide		
89	82736-95-6	1,2,4-Triazine-3,5(2H,4H)-dione, 6-fluoro-		
89	829-20-9	1-(2,4-Dimethoxyphenyl)ethan-1-one		
89	83173-76-6	Benzenemethanol, 4-methyl-à-(1-methyl-2-propenyl)-, (R*,R*)-		
89	85763-57-1	11-Methyldodecanol		
89	866-23-9	Phosphonic acid, trichloromethyl-, diethyl ester		
89	871-83-0	2-Methylnonane		
89	874-41-9	1,3-Dimethyl-4-ethylbenzene		
89	89656-98-4	Cyclohexane, (2-methyl-1-propenyl)-		
89	90565-51-8	2-butyl-4-methyl-1,6-dihydro-6-pyrimidone		
89	90832-26-1	4,5-Dihydro-à,à,4,4-tetramethyl-1H-pyrazole-1-propanol		
89	90921-72-5	N-Allyl-p-hydroxybenzamide		
89	91-17-8	Decalin		
89	91242-57-8	Cyclopentane, 1,2-dipropyl-		
89	92-51-3	Dicyclohexyl		
89	925-60-0	2-Propenoic acid, propyl ester		
89	931-36-2	2-Ethyl-4-methyl-1H-imidazole		
89	932-40-1	trans-1,2-Diethyl cyclopentane		
89	94492-10-1	2-Dimethylamino-4-methyl-pent-4-enenitrile		
89	95-65-8	3,4-Dimethylphenol		
89	96-76-4	2,4-Di-tert-butylphenol		
89	97-72-3	Isobutyric anhydride		
89	98060-54-9	Decane, trimethyl-		
89	99133-89-8	4-Imidazolacetic acid, butyl ester		
90	7440-09-7	Potassium	91.92	mg/L
90	14127-61-8	Calcium ion	2385.31	mg/L
90	14808-79-8	Sulfate	98.84	mg/L
90	15438-31-0	Fe +2 ion	56.11	mg/L
90	16887-00-6	Chloride	38414.67	mg/L
90	17341-25-2	Sodium ion	23548.9	mg/L
90	24959-67-9	Bromide	325.21	mg/L
90	7439-95-4	Magnesium	411.68	mg/L
90	7440-24-6	Strontium	1013.25	mg/L
90	7440-39-3	Barium	4225.49	mg/L
91	7439-96-5	Manganese		
91	7440-38-2	Arsenic		
91	7440-39-3	Barium		
91	7440-47-3	Chromium		
91	7440-50-8	Copper		
92	120-12-7	Anthracene	0.0017	mg/L
92	129-00-0	Pyrene		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
92	206-44-0	Fluoranthene		
92	218-01-9	Chrysene		
92	50-32-8	Benzo(a)pyrene	0.0021	mg/L
92	56-55-3	Benz(a)anthracene		
92	85-01-8	Phenanthrene	0.0683	mg/L
92	86-73-7	Fluorene	0.0407	mg/L
92	91-20-3	Naphthalene	0.359	mg/L
93	7440-09-7	Potassium	100	mg/L
93	14127-61-8	Calcium ion	480	mg/L
93	15438-31-0	Fe +2 ion	220	mg/L
93	16887-00-6	Chloride	24800	mg/L
93	17341-25-2	Sodium ion	15300	mg/L
93	24959-67-9	Bromide	135	mg/L
93	7439-93-2	Lithium	4.1	mg/L
93	7439-95-4	Magnesium	290	mg/L
93	7440-21-3	Silicon	12	mg/L
93	7440-39-3	Barium	190	mg/L
93	7440-42-8	Boron	9.3	mg/L
94	7440-09-7	Potassium	18	mg/L
94	14127-61-8	Calcium ion	69	mg/L
94	14808-79-8	Sulfate	17	mg/L
94	15438-31-0	Fe +2 ion	27	mg/L
94	16887-00-6	Chloride	64	mg/L
94	16984-48-8	Fluoride	1.7	mg/L
94	17341-25-2	Sodium ion	800	mg/L
94	22537-38-8	Rubidium, ion (Rb1+)	0.038	mg/L
94	24959-67-9	Bromide	12	mg/L
94	7439-92-1	Lead	0.00043	mg/L
94	7439-93-2	Lithium	0.208	mg/L
94	7439-95-4	Magnesium	46	mg/L
94	7439-96-5	Manganese	0.101	mg/L
94	7439-97-6	Mercury	0.00025	mg/L
94	7440-02-0	Nickel	0.035	mg/L
94	7440-20-2	Scandium	0.003	mg/L
94	7440-21-3	Silicon	7.1	mg/L
94	7440-24-6	Strontium	1.9	mg/L
94	7440-28-0	Thallium	0.00034	mg/L
94	7440-31-5	Tin	0.0055	mg/L
94	7440-38-2	Arsenic	0.0026	mg/L
94	7440-39-3	Barium	1.6	mg/L
94	7440-42-8	Boron	0.217	mg/L
94	7440-46-2	Cesium	0.00078	mg/L
94	7440-47-3	Chromium	0.0012	mg/L
94	7440-48-4	Cobalt	0.00022	mg/L
94	7440-50-8	Copper	0.029	mg/L
94	7440-62-2	Vanadium	0.00019	mg/L
94	7440-66-6	Zinc	0.08	mg/L
94	7440-69-9	Bismuth	0.032	mg/L
94	7664-41-7	Ammonia	5.3	mg/L
94	7723-14-0	Phosphorus	0.094	mg/L
95	10045-97-3	Caesium-137		
95	10098-97-2	Strontium-90		
95	10198-40-0	Cobalt 60		
95	13966-00-2	Potassium-40		
95	13966-02-4	Beryllium-7		
95	13967-63-0	Scandium-46		
95	13982-63-3	Radium-226		
95	14158-27-1	Strontium-89		
95	14255-04-0	Lead-210		
95	14274-82-9	Thorium 228		
95	14733-03-0	Bismuth-214		
95	14913-49-6	Bismuth-212		
95	14913-50-9	Thallium-208		
95	15067-28-4	Lead-214		
95	15117-96-1	Uranium-235		
95	15262-20-1	Radium-228		
96	7440-09-7	Potassium	526	mg/L
96	14127-61-8	Calcium ion	546	mg/L
96	16887-00-6	Chloride	20215	mg/L
96	17341-25-2	Sodium ion	9921	mg/L
96	24959-67-9	Bromide	227	mg/L
96	7439-93-2	Lithium	7.88	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
96	7439-95-4	Magnesium	70.5	mg/L
96	7440-21-3	Silicon	25.7	mg/L
96	7440-24-6	Strontium	72.5	mg/L
96	7440-39-3	Barium	38.1	mg/L
96	7440-42-8	Boron	22.8	mg/L
96	7704-34-9	Sulfur	10.6	mg/L
96	7723-14-0	Phosphorus	1.46	mg/L
97	7440-09-7	Potassium	48.4	mg/L
97	100-41-4	Ethylbenzene	0.074	mg/L
97	10098-97-2	Strontium-90	70.7	pCi/L
97	108-88-3	Toluene	0.152	mg/L
97	1330-20-7	Xylenes	0.017	mg/L
97	13982-63-3	Radium-226	4.5	pCi/L
97	15262-20-1	Radium-228	8.6	pCi/L
97	16887-00-6	Chloride	1500	mg/L
97	16984-48-8	Fluoride	0.94	mg/L
97	471-34-1	Carbonic acid calcium salt (1:1)	17000	mg/L
97	71-43-2	Benzene	0.072	mg/L
97	7439-89-6	Iron	4.2	mg/L
97	7439-92-1	Lead	0.27	mg/L
97	7439-95-4	Magnesium	33.9	mg/L
97	7440-23-5	Sodium	6532	mg/L
97	7440-38-2	Arsenic	0.011	mg/L
97	7440-39-3	Barium	61.9	mg/L
97	7440-42-8	Boron	2	mg/L
97	7440-66-6	Zinc	0.39	mg/L
97	7440-70-2	Calcium	56.1	mg/L
97	7782-49-2	Selenium	0.001	mg/L
98	7440-09-7	Potassium	54.7	mg/L
98	13982-63-3	Radium-226	85.13513514	pCi/L
98	14127-61-8	Calcium ion	266.9	mg/L
98	14255-04-0	Lead-210	1.162162162	pCi/L
98	14808-79-8	Sulfate	74.9	mg/L
98	16887-00-6	Chloride	11650	mg/L
98	17341-25-2	Sodium ion	6934	mg/L
98	24959-67-9	Bromide	168.5	mg/L
98	71-52-3	Bicarbonate	1303	mg/L
98	7429-90-5	Aluminum	3.3	mg/L
98	7439-89-6	Iron	69.3	mg/L
98	7439-95-4	Magnesium	38.4	mg/L
98	7439-96-5	Manganese	0.97	mg/L
98	7440-21-3	Silicon	48.8	mg/L
98	7440-24-6	Strontium	40	mg/L
98	7440-39-3	Barium	14.2	mg/L
99	100-41-4	Ethylbenzene	1.54	mg/L
99	100-42-5	Styrene	0.0359	mg/L
99	103-65-1	Propylbenzene	0.465	mg/L
99	104-51-8	Butylbenzene	0.0735	mg/L
99	108-10-1	4-Methyl-2-pentanone	1.44	mg/L
99	108-67-8	1,3,5-Trimethylbenzene	0.73	mg/L
99	108-88-3	Toluene	41.5	mg/L
99	122-20-3	Triisopropanolamine		
99	135-98-8	sec-Butylbenzene	2.02	mg/L
99	179601-23-1	m,p-Xylene	52.5	mg/L
99	591-78-6	2-Hexanone	1.07	mg/L
99	67-64-1	Acetone	21.7	mg/L
99	71-43-2	Benzene	12.5	mg/L
99	78-93-3	Methyl ethyl ketone	0.199	mg/L
99	95-47-6	o-Xylene	20.5	mg/L
99	95-63-6	1,2,4-Trimethylbenzene	2.29	mg/L
99	98-06-6	tert-Butylbenzene	0.256	mg/L
99	99-87-6	p-Cymene	0.0906	mg/L
100	7440-09-7	Potassium	75.9	mg/L
100	14265-44-2	Phosphate	7.2	mg/L
100	14808-79-8	Sulfate	26.63	mg/L
100	16887-00-6	Chloride	27103	mg/L
100	24959-67-9	Bromide	265.1	mg/L
100	5579-66-8	3,6,9,12,15,18,21,24,27-Nonaoxanonacosane-1,29-diol		
100	7439-89-6	Iron	19	mg/L
100	7439-95-4	Magnesium	130	mg/L
100	7439-96-5	Manganese	89.9	mg/L
100	7440-21-3	Silicon	42	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
100	7440-23-5	Sodium	14794	mg/L
100	7440-24-6	Strontium	202	mg/L
100	7440-39-3	Barium	41.39	mg/L
100	7440-70-2	Calcium	1204.2	mg/L
101	12587-46-1	Alpha particle	123000	pCi/L
101	12587-47-2	Beta particle	12000	pCi/L
101	13982-63-3	Radium-226	16920	pCi/L
101	15262-20-1	Radium-228	2589	pCi/L
101	7440-14-4	Radium	18045	pCi/L
102	7440-09-7	Potassium	1210	mg/L
102	14701-22-5	Nickel cation	19.2	mg/L
102	14808-79-8	Sulfate	774	mg/L
102	16887-00-6	Chloride	184000	mg/L
102	24959-67-9	Bromide	1470	mg/L
102	71-52-3	Bicarbonate	364	mg/L
102	7439-89-6	Iron	519	mg/L
102	7439-92-1	Lead	1.09	mg/L
102	7439-93-2	Lithium	282	mg/L
102	7439-95-4	Magnesium	3670	mg/L
102	7439-96-5	Manganese	26.6	mg/L
102	7440-17-7	Rubidium	1.39	mg/L
102	7440-23-5	Sodium	63100	mg/L
102	7440-24-6	Strontium	10300	mg/L
102	7440-39-3	Barium	22400	mg/L
102	7440-42-8	Boron	47.3	mg/L
102	7440-46-2	Cesium	0.358	mg/L
102	7440-48-4	Cobalt	0.039	mg/L
102	7440-50-8	Copper	1.57	mg/L
102	7440-66-6	Zinc	2.17	mg/L
102	7440-70-2	Calcium	39200	mg/L
102	7553-56-2	Iodine	29.9	mg/L
103	7440-09-7	Potassium	27.91	mg/L
103	14797-55-8	Nitrate	1.9	mg/L
103	14808-79-8	Sulfate	123.35	mg/L
103	16887-00-6	Chloride	12717	mg/L
103	7439-89-6	Iron	0.08	mg/L
103	7439-92-1	Lead	0.03	mg/L
103	7439-95-4	Magnesium	35.07	mg/L
103	7440-23-5	Sodium	7602	mg/L
103	7440-39-3	Barium	3.36	mg/L
103	7440-42-8	Boron	14.8	mg/L
103	7440-70-2	Calcium	169.12	mg/L
103	7782-49-2	Selenium	0.202	mg/L
104	14797-55-8	Nitrate	2.25	mg/L
104	14808-79-8	Sulfate	69.95	mg/L
104	16887-00-6	Chloride	20606	mg/L
104	17341-25-2	Sodium ion	8769	mg/L
104	7439-89-6	Iron	5	mg/L
104	7440-39-3	Barium	49	mg/L
104	7440-42-8	Boron	123	mg/L
104	7440-70-2	Calcium	1038	mg/L
104	7631-86-9	Silica	185	mg/L
104	7664-41-7	Ammonia	0.4	mg/L
104	7723-14-0	Phosphorus	1.19	mg/L
105	24959-67-9	Bromide	1120	mg/L
105	7439-89-6	Iron	370	mg/L
105	7439-92-1	Lead	31.4	mg/L
105	7439-96-5	Manganese	62	mg/L
105	7439-98-7	Molybdenum	0.05	mg/L
105	7440-22-4	Silver	0.009	mg/L
105	7440-24-6	Strontium	1600	mg/L
105	7440-28-0	Thallium	0.21	mg/L
105	7440-38-2	Arsenic	0.35	mg/L
105	7440-42-8	Boron	180	mg/L
105	7440-43-9	Cadmium	0.82	mg/L
105	7440-46-2	Cesium	0.58	mg/L
105	7440-48-4	Cobalt	0.22	mg/L
105	7440-50-8	Copper	0.37	mg/L
105	7440-57-5	Gold	0.018	mg/L
105	7440-61-1	Uranium	0.09	mg/L
105	7440-66-6	Zinc	174	mg/L
106	7440-09-7	Potassium	1050	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
106	7446-09-5	Sulfur dioxide	0.03225	mg/L
106	100-01-6	4-Nitroaniline	0.0026	mg/L
106	100-41-4	Ethylbenzene	0.00693	mg/L
106	10045-97-3	Caesium-137	9	pCi/L
106	10098-97-2	Strontium-90	0.44	pCi/L
106	104-76-7	2-Ethyl-1-hexanol	0.041	mg/L
106	105-67-9	2,4-Dimethylphenol	0.00039	mg/L
106	106-46-7	1,4-Dichlorobenzene	0.00034	mg/L
106	107-21-1	Ethylene glycol	290	mg/L
106	108-10-1	4-Methyl-2-pentanone	0.00065	mg/L
106	108-38-3	m-Xylene	0.111	mg/L
106	108-67-8	1,3,5-Trimethylbenzene	0.0034	mg/L
106	108-88-3	Toluene	2.3	mg/L
106	108-95-2	Phenol	0.084	mg/L
106	110-86-1	Pyridine	0.28	mg/L
106	1120-21-4	Undecane	0.0113	mg/L
106	112-30-1	1-Decanol	0.0054	mg/L
106	112-40-3	Dodecane	0.0706	mg/L
106	117-81-7	Di(2-ethylhexyl) phthalate	0.0091	mg/L
106	117-84-0	Di-n-octyl phthalate	0.0093	mg/L
106	118-74-1	Hexachlorobenzene	0.001	mg/L
106	119-64-2	Tetralin	0.00895	mg/L
106	120-82-1	1,2,4-Trichlorobenzene	0.0015	mg/L
106	122-39-4	Diphenylamine	0.0017	mg/L
106	123-91-1	1,4-Dioxane	0.0095	mg/L
106	124-38-9	Carbon dioxide	0.29	mg/L
106	12587-46-1	Alpha particle	40880	pCi/L
106	12587-47-2	Beta particle	216740.95	pCi/L
106	127-18-4	Tetrachloroethylene	0.005	mg/L
106	131-11-3	Dimethyl phthalate	0.0015	mg/L
106	1330-20-7	Xylenes	0.064	mg/L
106	13966-00-2	Potassium-40	700	pCi/L
106	13966-29-5	Uranium 234	22.1	pCi/L
106	13982-63-3	Radium-226	16920	pCi/L
106	14255-04-0	Lead-210	310	pCi/L
106	14265-45-3	Sulfite	9.2	mg/L
106	14269-63-7	Thorium 230	6.9	pCi/L
106	14274-82-9	Thorium 228	45.9	pCi/L
106	14331-83-0	Actinium 228	1180	pCi/L
106	14331-85-2	protactinium-231	240	pCi/L
106	14733-03-0	Bismuth-214	7330	pCi/L
106	14797-55-8	Nitrate	1.4	mg/L
106	14797-65-0	Nitrite	219	mg/L
106	14808-79-8	Sulfate	671	mg/L
106	14913-49-6	Bismuth-212	150	pCi/L
106	14913-50-9	Thallium-208	0.4	pCi/L
106	14952-40-0	Actinium-227	2	pCi/L
106	15065-10-8	Thorium 234	170	pCi/L
106	15067-28-4	Lead-214	7350	pCi/L
106	15092-94-1	Lead-212	54	pCi/L
106	15100-28-4	Protactinium-234	1400	pCi/L
106	15117-96-1	Uranium-235	40	pCi/L
106	15229-37-5	Bismuth-211	2	pCi/L
106	15262-20-1	Radium-228	3089	pCi/L
106	1560-97-0	2-Methyldodecane	0.0097	mg/L
106	15623-45-7	Radium-223	2	pCi/L
106	15623-47-9	Thorium 227	3	pCi/L
106	156-60-5	(E)-1,2-Dichloroethylene	0.005	mg/L
106	16065-83-1	Chromium (III)	0.0447	mg/L
106	16887-00-6	Chloride	192000	mg/L
106	1718-52-1	Perdeuteriopyrene	0.0011	mg/L
106	17301-23-4	2,6-Dimethylundecane	0.2018	mg/L
106	17312-57-1	3-Methyldodecane	0.0049	mg/L
106	1758-88-9	2-Ethyl-p-xylene	0.3469	mg/L
106	18496-25-8	Sulfide	4	mg/L
106	18540-29-9	Chromium (VI) ion	5.4	mg/L
106	191-24-2	Benzo(g,h,i)perylene	0.0012	mg/L
106	193-39-5	Indeno(1,2,3-cd)pyrene	0.0024	mg/L
106	205-99-2	Benzo(b)fluoranthene	0.001	mg/L
106	206-44-0	Fluoranthene	0.0013	mg/L
106	207-08-9	Benzo(k)fluoranthene	0.00091	mg/L
106	218-01-9	Chrysene	0.0011	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
106	24959-67-9	Bromide	3340	mg/L
106	25415-84-3	Butanoic acid, 2-ethylhexyl ester	0.0004	mg/L
106	2658-24-4	2,2-Dimethylaziridine	0.0002	mg/L
106	319-86-8	delta-Hexachlorocyclohexane	0.000048	mg/L
106	32038-83-8	2-Propynenitrile, 3-fluoro-	0.00018	mg/L
106	496-11-7	Indan	0.0096	mg/L
106	50-32-8	Benzo(a)pyrene	0.0011	mg/L
106	53-70-3	Dibenz(a,h)anthracene	0.0023	mg/L
106	541-73-1	1,3-Dichlorobenzene	0.0003	mg/L
106	56-55-3	Benz(a)anthracene	0.0012	mg/L
106	57-12-5	Cyanide	0.1	mg/L
106	57-55-6	1,2-Propylene glycol	110	mg/L
106	59473-04-0	Tox	3.88	mg/L
106	6032-29-7	Pentan-2-ol	0.0087	mg/L
106	611-14-3	1-Ethyl-2-methylbenzene	0.0061	mg/L
106	6117-97-1	4-Methyldodecane	0.0101	mg/L
106	629-50-5	Tridecane	0.0524	mg/L
106	629-59-4	Tetradecane	0.016	mg/L
106	64-17-5	Ethanol	0.5333	mg/L
106	64-19-7	Acetic acid	6.6	mg/L
106	67-56-1	Methanol	428	mg/L
106	67-63-0	Isopropanol	83	mg/L
106	67-64-1	Acetone	0.21	mg/L
106	700-12-9	Benzene, pentamethyl-	0.2588	mg/L
106	7045-71-8	2-Methylundecane	0.0703	mg/L
106	71-43-2	Benzene	1.345	mg/L
106	7429-90-5	Aluminum	686	mg/L
106	7439-89-6	Iron	1390	mg/L
106	7439-92-1	Lead	3.6	mg/L
106	7439-93-2	Lithium	633.925	mg/L
106	7439-95-4	Magnesium	3670	mg/L
106	7439-96-5	Manganese	48.5	mg/L
106	7439-97-6	Mercury	0.0079	mg/L
106	7439-98-7	Molybdenum	1.5	mg/L
106	7439-99-8	Neptunium	1640	pCi/L
106	7440-02-0	Nickel	3.2	mg/L
106	7440-21-3	Silicon	49.29	mg/L
106	7440-22-4	Silver	0.093	mg/L
106	7440-23-5	Sodium	81800	mg/L
106	7440-24-6	Strontium	15400	mg/L
106	7440-28-0	Thallium	0.0564	mg/L
106	7440-29-1	Thorium	35.9	mg/L
106	7440-31-5	Tin	0.052	mg/L
106	7440-32-6	Titanium	0.148	mg/L
106	7440-36-0	Antimony	0.0491	mg/L
106	7440-38-2	Arsenic	1.1	mg/L
106	7440-39-3	Barium	15000	mg/L
106	7440-41-7	Beryllium	0.0022	mg/L
106	7440-42-8	Boron	94.7	mg/L
106	7440-43-9	Cadmium	0.018	mg/L
106	7440-44-0	Carbon	3750	mg/L
106	7440-47-3	Chromium	2.2	mg/L
106	7440-48-4	Cobalt	2.36	mg/L
106	7440-50-8	Copper	18	mg/L
106	7440-61-1	Uranium	170	pCi/L
106	7440-66-6	Zinc	17.1	mg/L
106	7440-70-2	Calcium	43400	mg/L
106	74-87-3	Chloromethane	0.0054	mg/L
106	75-09-2	Dichloromethane	0.0118	mg/L
106	75163-97-2	octadecane, 2,6-dimethyl-	0.2917	mg/L
106	75-34-3	1,1-Dichloroethane	0.005	mg/L
106	75-83-2	2,2-Dimethylbutane	0.00066	mg/L
106	7631-86-9	Silica	36.5	mg/L
106	7664-41-7	Ammonia	409	mg/L
106	7723-14-0	Phosphorus	4222	mg/L
106	7727-37-9	Nitrogen	96026	mg/L
106	7782-49-2	Selenium	0.17	mg/L
106	78-93-3	Methyl ethyl ketone	0.018	mg/L
106	83-32-9	Acenaphthene	0.00029	mg/L
106	84-66-2	Diethyl phthalate	0.0026	mg/L
106	84-74-2	Dibutyl phthalate	0.0015	mg/L
106	85-01-8	Phenanthrene	0.0013	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
106	86-30-6	N-Nitrosodiphenylamine	0.0017	mg/L
106	86-73-7	Fluorene	0.0014	mg/L
106	87-61-6	1,2,3-Trichlorobenzene	0.0065	mg/L
106	91-20-3	Naphthalene	0.0028	mg/L
106	91-57-6	2-Methylnaphthalene	0.00995	mg/L
106	95-48-7	o-Cresol	0.00021	mg/L
106	95-50-1	1,2-Dichlorobenzene	0.00068	mg/L
106	95-63-6	1,2,4-Trimethylbenzene	0.0042	mg/L
106	959-98-8	Endosulfan I	0.0005	mg/L
106	98-86-2	Acetophenone	0.0011	mg/L
107	7440-09-7	Potassium	173	mg/L
107	16887-00-6	Chloride	90292	mg/L
107	7429-90-5	Aluminum	0.38	mg/L
107	7439-89-6	Iron	45	mg/L
107	7439-92-1	Lead	1.5	mg/L
107	7439-95-4	Magnesium	2509	mg/L
107	7440-23-5	Sodium	53381	mg/L
107	7440-24-6	Strontium	291	mg/L
107	7440-39-3	Barium	396	mg/L
107	7440-66-6	Zinc	1.2	mg/L
107	7440-70-2	Calcium	10577	mg/L
108	7440-09-7	Potassium	125.43	mg/L
108	14808-79-8	Sulfate	1745.27	mg/L
108	16887-00-6	Chloride	5885.37	mg/L
108	71-52-3	Bicarbonate	1189.1	mg/L
108	7439-89-6	Iron	0.097	mg/L
108	7439-95-4	Magnesium	330.52	mg/L
108	7440-23-5	Sodium	2902.71	mg/L
108	7440-42-8	Boron	31.6	mg/L
108	7440-70-2	Calcium	1240.09	mg/L
108	7631-86-9	Silica	172	mg/L
109	7440-09-7	Potassium	670	mg/L
109	100-41-4	Ethylbenzene	0.016	mg/L
109	100-42-5	Styrene	0.001	mg/L
109	103-65-1	Propylbenzene	0.007	mg/L
109	104-51-8	Butylbenzene	0.01	mg/L
109	105-67-9	2,4-Dimethylphenol	0.008	mg/L
109	106-42-3	p-Xylene	0.033	mg/L
109	107-92-6	Butanoic acid	1.776	mg/L
109	108-38-3	m-Xylene	0.022	mg/L
109	108-67-8	1,3,5-Trimethylbenzene	0.01	mg/L
109	108-88-3	Toluene	0.202	mg/L
109	110-75-8	2-Chloroethyl vinyl ether	0.014	mg/L
109	120-12-7	Anthracene	0.001	mg/L
109	142-62-1	Hexanoic acid	0.216	mg/L
109	14808-79-8	Sulfate	1.6	mg/L
109	16887-00-6	Chloride	103000	mg/L
109	24959-67-9	Bromide	342	mg/L
109	503-74-2	Isovaleric acid	0.96	mg/L
109	64-19-7	Acetic acid	6.48	mg/L
109	646-07-1	Pentanoic acid, 4-methyl-	3.456	mg/L
109	71-43-2	Benzene	0.531	mg/L
109	7439-89-6	Iron	47.1	mg/L
109	7439-93-2	Lithium	31.6	mg/L
109	7439-95-4	Magnesium	2440	mg/L
109	7439-96-5	Manganese	5.7	mg/L
109	7440-23-5	Sodium	50000	mg/L
109	7440-24-6	Strontium	827	mg/L
109	7440-39-3	Barium	468	mg/L
109	7440-47-3	Chromium	0.03	mg/L
109	7440-70-2	Calcium	10700	mg/L
109	79-09-4	Propionic acid	0.324	mg/L
109	79-31-2	2-Methylpropanoic acid	0.384	mg/L
109	79-34-5	1,1,2,2-Tetrachloroethane	0.005	mg/L
109	80-62-6	Methyl methacrylate	0.03	mg/L
109	90-12-0	1-Methylnaphthalene	0.003	mg/L
109	91-20-3	Naphthalene	0.025	mg/L
109	95-47-6	o-Xylene	0.045	mg/L
109	95-63-6	1,2,4-Trimethylbenzene	0.003	mg/L
109	98-82-8	Cumene	0.064	mg/L
109	98-95-3	Nitrobenzene	0.006	mg/L
109	99-87-6	p-Cymene	0.005	mg/L
110	7440-09-7	Potassium	163	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
110	1120-21-4	Undecane		
110	112-40-3	Dodecane		
110	124-18-5	Decane		
110	14808-79-8	Sulfate	15.17	mg/L
110	16887-00-6	Chloride	39579	mg/L
110	24959-67-9	Bromide	428.2	mg/L
110	295-17-0	Cyclotetradecane		
110	544-76-3	Hexadecane		
110	629-50-5	Tridecane		
110	629-59-4	Tetradecane		
110	7429-90-5	Aluminum	0.1366	mg/L
110	7439-89-6	Iron	13.7	mg/L
110	7439-92-1	Lead	0.0066	mg/L
110	7439-93-2	Lithium	38	mg/L
110	7439-95-4	Magnesium	2.17	mg/L
110	7439-96-5	Manganese	483	mg/L
110	7439-98-7	Molybdenum	0.02231	mg/L
110	7440-02-0	Nickel	0.00992	mg/L
110	7440-17-7	Rubidium	0.4501	mg/L
110	7440-21-3	Silicon	27.6	mg/L
110	7440-23-5	Sodium	18600	mg/L
110	7440-24-6	Strontium	844	mg/L
110	7440-28-0	Thallium	0.00115	mg/L
110	7440-29-1	Thorium	0.00511	mg/L
110	7440-31-5	Tin	0.3341	mg/L
110	7440-36-0	Antimony	0.00827	mg/L
110	7440-38-2	Arsenic	0.04254	mg/L
110	7440-39-3	Barium	861	mg/L
110	7440-43-9	Cadmium	0.0009	mg/L
110	7440-46-2	Cesium	0.1226	mg/L
110	7440-47-3	Chromium	0.00517	mg/L
110	7440-48-4	Cobalt	0.0011	mg/L
110	7440-50-8	Copper	0.1862	mg/L
110	7440-58-6	Hafnium	0.00545	mg/L
110	7440-61-1	Uranium	0.0012	mg/L
110	7440-62-2	Vanadium	0.00211	mg/L
110	7440-66-6	Zinc	1.01	mg/L
110	7440-70-2	Calcium	4650	mg/L
110	7723-14-0	Phosphorus	3.43	mg/L
110	7782-49-2	Selenium	0.00767	mg/L
111	14808-79-8	Sulfate	77	mg/L
111	7439-89-6	Iron	45	mg/L
112	14797-55-8	Nitrate	34.99	mg/L
112	16887-00-6	Chloride	500	mg/L
112	16984-48-8	Fluoride	1.38	mg/L
112	471-34-1	Carbonic acid calcium salt (1:1)	315	mg/L
112	7439-89-6	Iron	0.45	mg/L
112	7439-95-4	Magnesium	41.92	mg/L
112	7439-96-5	Manganese	2	mg/L
112	7440-23-5	Sodium	570	mg/L
112	7440-70-2	Calcium	57	mg/L
112	7553-56-2	Iodine	0.4	mg/L
114	7440-09-7	Potassium	1650	mg/L
114	7783-06-4	Hydrogen sulfide	600	mg/L
114	14808-79-8	Sulfate	1750	mg/L
114	16887-00-6	Chloride	122450	mg/L
114	471-34-1	Carbonic acid calcium salt (1:1)	740	mg/L
114	7439-95-4	Magnesium	2160	mg/L
114	7439-97-6	Mercury	0.0071	mg/L
114	7440-22-4	Silver	0.02	mg/L
114	7440-23-5	Sodium	59900	mg/L
114	7440-39-3	Barium	0.3	mg/L
114	7440-47-3	Chromium	0.8	mg/L
114	7440-70-2	Calcium	1750	mg/L
114	7723-14-0	Phosphorus	6	mg/L
114	7727-37-9	Nitrogen	30	mg/L
114	7782-49-2	Selenium	0.001	mg/L
115	108-88-3	Toluene		
115	111-76-2	2-Butoxyethanol		
115	112-18-5	N,N-Dimethyldodecan-1-amine		
115	112-75-4	N,N-Dimethyltetradecylamine		
115	14797-55-8	Nitrate	2670	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
115	14808-79-8	Sulfate	5590	mg/L
115	16887-00-6	Chloride	216000	mg/L
115	16984-48-8	Fluoride	33	mg/L
115	24959-67-9	Bromide	10600	mg/L
115	7439-89-6	Iron	2838	mg/L
115	7439-98-7	Molybdenum	5.06	mg/L
115	7440-02-0	Nickel	4.78	mg/L
115	7440-24-6	Strontium	1310	mg/L
115	7440-32-6	Titanium	4.16	mg/L
115	7440-39-3	Barium	4370	mg/L
115	7440-41-7	Beryllium	0.266	mg/L
115	7440-47-3	Chromium	2.33	mg/L
115	7440-48-4	Cobalt	4.14	mg/L
115	7440-50-8	Copper	15	mg/L
115	7440-62-2	Vanadium	4.51	mg/L
115	7440-66-6	Zinc	20	mg/L
115	7440-67-7	Zirconium	8.76	mg/L
115	74-87-3	Chloromethane		
115	75-15-0	Carbon disulfide		
115	95-47-6	o-Xylene		
116	7440-09-7	Potassium	1100	mg/L
116	14127-61-8	Calcium ion	23000	mg/L
116	14808-79-8	Sulfate	1500	mg/L
116	16887-00-6	Chloride	157000	mg/L
116	17341-25-2	Sodium ion	54000	mg/L
116	18496-25-8	Sulfide	7700	mg/L
116	24959-67-9	Bromide	1820	mg/L
116	71-52-3	Bicarbonate	160	mg/L
116	7439-89-6	Iron	120	mg/L
116	7439-93-2	Lithium	369	mg/L
116	7439-95-4	Magnesium	1950	mg/L
116	7439-96-5	Manganese	53	mg/L
116	7440-39-3	Barium	9700	mg/L
116	7440-48-4	Cobalt	8.2	mg/L
117	25322-69-4	Polypropylene glycol		
118	25322-68-3	Polyethylene glycol		
118	25322-69-4	Polypropylene glycol		
119	7440-09-7	Potassium		
119	100-41-4	Ethylbenzene		
119	100-51-6	Benzyl alcohol		
119	104-51-8	Butylbenzene		
119	105-67-9	2,4-Dimethylphenol		
119	106-44-5	p-Cresol		
119	107-92-6	Butanoic acid		
119	108-39-4	m-Cresol		
119	108-67-8	1,3,5-Trimethylbenzene		
119	108-88-3	Toluene		
119	108-95-2	Phenol		
119	109-52-4	Pentanoic acid		
119	110-86-1	Pyridine		
119	111-14-8	Heptanoic acid		
119	117-81-7	Di(2-ethylhexyl) phthalate		
119	117-84-0	Di-n-octyl phthalate		
119	123-91-1	1,4-Dioxane		
119	124-38-9	Carbon dioxide		
119	128-39-2	2,6-Di-tert-butylphenol		
119	129-00-0	Pyrene		
119	1330-20-7	Xylenes		
119	13982-63-3	Radium-226		
119	142-62-1	Hexanoic acid		
119	14797-55-8	Nitrate		
119	14797-65-0	Nitrite		
119	14808-79-8	Sulfate		
119	15262-20-1	Radium-228		
119	16887-00-6	Chloride		
119	16984-48-8	Fluoride		
119	18540-29-9	Chromium (VI) ion		
119	191-24-2	Benzo(g,h,i)perylene		
119	24959-67-9	Bromide		
119	503-74-2	Isovaleric acid		
119	57-12-5	Cyanide		
119	64-18-6	Formic acid		

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
119	64-19-7	Acetic acid		
119	67-64-1	Acetone		
119	67-66-3	Chloroform		
119	71-43-2	Benzene		
119	7429-90-5	Aluminum		
119	7439-89-6	Iron		
119	7439-92-1	Lead		
119	7439-93-2	Lithium		
119	7439-95-4	Magnesium		
119	7439-96-5	Manganese		
119	7439-97-6	Mercury		
119	7439-98-7	Molybdenum		
119	7440-02-0	Nickel		
119	7440-21-3	Silicon		
119	7440-22-4	Silver		
119	7440-23-5	Sodium		
119	7440-24-6	Strontium		
119	7440-28-0	Thallium		
119	7440-31-5	Tin		
119	7440-32-6	Titanium		
119	7440-36-0	Antimony		
119	7440-38-2	Arsenic		
119	7440-39-3	Barium		
119	7440-41-7	Beryllium		
119	7440-42-8	Boron		
119	7440-43-9	Cadmium		
119	7440-47-3	Chromium		
119	7440-48-4	Cobalt		
119	7440-50-8	Copper		
119	7440-62-2	Vanadium		
119	7440-66-6	Zinc		
119	7440-67-7	Zirconium		
119	7440-70-2	Calcium		
119	74-87-3	Chloromethane		
119	75-09-2	Dichloromethane		
119	75-25-2	Bromoform		
119	7631-86-9	Silica		
119	7664-41-7	Ammonia		
119	7782-49-2	Selenium		
119	78-93-3	Methyl ethyl ketone		
119	79-09-4	Propionic acid		
119	79-31-2	2-Methylpropanoic acid		
119	84-74-2	Dibutyl phthalate		
119	85-01-8	Phenanthrene		
119	86-30-6	N-Nitrosodiphenylamine		
119	86-73-7	Fluorene		
119	91-20-3	Naphthalene		
119	91-57-6	2-Methylnaphthalene		
119	95-48-7	o-Cresol		
119	95-63-6	1,2,4-Trimethylbenzene		
119	99-87-6	p-Cymene		
119	NOCAS_24858	m,p-Cresol mixture		
120	14127-61-8	Calcium ion	6360	mg/L
120	14808-79-8	Sulfate	71.5	mg/L
120	16887-00-6	Chloride	37600	mg/L
120	17341-25-2	Sodium ion	18300	mg/L
120	7439-89-6	Iron	18.3	mg/L
120	7439-95-4	Magnesium	449	mg/L
120	7439-96-5	Manganese	2	mg/L
120	7440-24-6	Strontium	1051.3	mg/L
120	7440-39-3	Barium	62.5	mg/L
121	14808-79-8	Sulfate	66.53	mg/L
121	15438-31-0	Fe +2 ion	4.22	mg/L
121	16887-00-6	Chloride	33000	mg/L
121	17341-25-2	Sodium ion	17060	mg/L
121	7439-95-4	Magnesium	373	mg/L
121	7440-24-6	Strontium	1051	mg/L
121	7440-39-3	Barium	1386	mg/L
121	7440-70-2	Calcium	3688	mg/L
122	14127-61-8	Calcium ion	37000	mg/L
122	16887-00-6	Chloride	162400	mg/L
122	17341-25-2	Sodium ion	64000	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
122	24959-67-9	Bromide	1900	mg/L
122	7439-93-2	Lithium	139	mg/L
122	7439-95-4	Magnesium	6000	mg/L
122	7440-24-6	Strontium	5000	mg/L
122	7440-39-3	Barium	3100	mg/L
122	7440-42-8	Boron	62.6	mg/L
123	13982-63-3	Radium-226	260	pCi/L
123	14808-79-8	Sulfate	3	mg/L
123	15262-20-1	Radium-228	34	pCi/L
123	16887-00-6	Chloride	12287	mg/L
123	17341-25-2	Sodium ion	4607	mg/L
123	24959-67-9	Bromide	144	mg/L
123	7439-89-6	Iron	13	mg/L
123	7439-93-2	Lithium	28.145	mg/L
123	7439-95-4	Magnesium	75	mg/L
123	7439-96-5	Manganese	3	mg/L
123	7440-21-3	Silicon	160	mg/L
123	7440-24-6	Strontium	49	mg/L
123	7440-39-3	Barium	5	mg/L
123	7440-42-8	Boron	21.102	mg/L
123	7440-70-2	Calcium	386	mg/L
124	7440-09-7	Potassium	2440	mg/L
124	100-41-4	Ethylbenzene	19.5	mg/L
124	100-42-5	Styrene	0.119	mg/L
124	100-51-6	Benzyl alcohol	0.34	mg/L
124	105-67-9	2,4-Dimethylphenol	0.36	mg/L
124	106-44-5	p-Cresol	0.3	mg/L
124	108-88-3	Toluene	37.2	mg/L
124	108-95-2	Phenol	0.77	mg/L
124	112-40-3	Dodecane	2.33	mg/L
124	112-95-8	Eicosane	0.222	mg/L
124	117-81-7	Di(2-ethylhexyl) phthalate	0.042	mg/L
124	124-18-5	Decane	2.67	mg/L
124	132-65-0	Dibenzothiophene	0.0144	mg/L
124	1330-20-7	Xylenes	11	mg/L
124	16887-00-6	Chloride	200000	mg/L
124	16984-48-8	Fluoride	4.6	mg/L
124	18496-25-8	Sulfide	6	mg/L
124	544-76-3	Hexadecane	0.601	mg/L
124	593-45-3	Octadecane	0.28	mg/L
124	629-59-4	Tetradecane	0.948	mg/L
124	629-97-0	Docosane	0.224	mg/L
124	630-01-3	Hexacosane	0.0651	mg/L
124	630-02-4	Octacosane	0.0387	mg/L
124	638-68-6	Triacontane	0.0131	mg/L
124	646-31-1	Tetracosane	0.112	mg/L
124	65-85-0	Benzoic acid	0.24	mg/L
124	67-64-1	Acetone	16	mg/L
124	71-43-2	Benzene	27.5	mg/L
124	7429-90-5	Aluminum	0.011	mg/L
124	7439-89-6	Iron	0.34	mg/L
124	7439-92-1	Lead	0.001	mg/L
124	7439-93-2	Lithium	1230	mg/L
124	7439-95-4	Magnesium	2.7	mg/L
124	7439-96-5	Manganese	0.065	mg/L
124	7440-02-0	Nickel	0.00007	mg/L
124	7440-21-3	Silicon	38.2	mg/L
124	7440-22-4	Silver	0.000004	mg/L
124	7440-23-5	Sodium	42.7	mg/L
124	7440-24-6	Strontium	6340	mg/L
124	7440-31-5	Tin	0.0032	mg/L
124	7440-36-0	Antimony	0.00027	mg/L
124	7440-38-2	Arsenic	0.0024	mg/L
124	7440-39-3	Barium	0.86	mg/L
124	7440-42-8	Boron	0.14	mg/L
124	7440-47-3	Chromium	0.001	mg/L
124	7440-62-2	Vanadium	0.0006	mg/L
124	7440-66-6	Zinc	0.028	mg/L
124	7440-70-2	Calcium	30	mg/L
124	7553-56-2	Iodine	34	mg/L
124	7664-41-7	Ammonia	350	mg/L
124	7704-34-9	Sulfur	112	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
124	7723-14-0	Phosphorus	4.06	mg/L
124	78-59-1	Isophorone	0.015	mg/L
124	78-93-3	Methyl ethyl ketone	0.51	mg/L
124	79-01-6	Trichloroethylene	2.68	mg/L
124	83-32-9	Acenaphthene	0.0023	mg/L
124	84-74-2	Dibutyl phthalate	0.0151	mg/L
124	85-01-8	Phenanthrene	0.034	mg/L
124	91-20-3	Naphthalene	0.12	mg/L
124	91-57-6	2-Methylnaphthalene	0.13	mg/L
124	92-52-4	Biphenyl	0.0242	mg/L
124	95-48-7	o-Cresol	0.56	mg/L
124	99-87-6	p-Cymene	0.16	mg/L
125	13982-63-3	Radium-226	2510	pCi/L
125	16887-00-6	Chloride	66200	mg/L
125	17341-25-2	Sodium ion	28400	mg/L
125	7440-39-3	Barium	297	mg/L
126	13982-63-3	Radium-226	833	pCi/L
126	15262-20-1	Radium-228	814.8648649	pCi/L
127	7440-09-7	Potassium	260.06	mg/L
127	100-41-4	Ethylbenzene	52.52	mg/L
127	100-42-5	Styrene	10.85	mg/L
127	108-88-3	Toluene	621.71	mg/L
127	14127-61-8	Calcium ion	7269.23	mg/L
127	14265-44-2	Phosphate	8.03	mg/L
127	14797-55-8	Nitrate	0.02	mg/L
127	14797-65-0	Nitrite	0.06	mg/L
127	14808-79-8	Sulfate	38.7	mg/L
127	16887-00-6	Chloride	42683.1	mg/L
127	179601-23-1	m,p-Xylene	698.71	mg/L
127	24959-67-9	Bromide	465.96	mg/L
127	71-43-2	Benzene	149.59	mg/L
127	7429-90-5	Aluminum	1.4	mg/L
127	7439-89-6	Iron	67.1	mg/L
127	7439-92-1	Lead	0.01	mg/L
127	7439-95-4	Magnesium	835	mg/L
127	7439-96-5	Manganese	5.5	mg/L
127	7440-23-5	Sodium	26202.31	mg/L
127	7440-24-6	Strontium	1365.38	mg/L
127	7440-39-3	Barium	514.68	mg/L
127	7440-47-3	Chromium	0.03	mg/L
127	7440-66-6	Zinc	0.1	mg/L
127	74-82-8	Methane	3420.48	mg/L
127	74-84-0	Ethane	571.19	mg/L
127	74-98-6	Propane	86.92	mg/L
127	7704-34-9	Sulfur	36.16	mg/L
127	7782-49-2	Selenium	0.06	mg/L
127	95-47-6	o-Xylene	142.27	mg/L
128	7440-09-7	Potassium	488	mg/L
128	100-41-4	Ethylbenzene	0.235	mg/L
128	100-42-5	Styrene	0.141	mg/L
128	108-88-3	Toluene	2.45	mg/L
128	12587-46-1	Alpha particle	20920	pCi/L
128	12587-47-2	Beta particle	4664	pCi/L
128	13966-00-2	Potassium-40	221	pCi/L
128	13982-63-3	Radium-226	1194	pCi/L
128	14127-61-8	Calcium ion	19900	mg/L
128	14265-44-2	Phosphate	90	mg/L
128	14269-63-7	Thorium 230	9.37	pCi/L
128	14274-82-9	Thorium 228	2.35	pCi/L
128	14797-55-8	Nitrate	0.3	mg/L
128	14797-65-0	Nitrite	0.8	mg/L
128	14808-79-8	Sulfate	108	mg/L
128	15262-20-1	Radium-228	216	pCi/L
128	16887-00-6	Chloride	79000	mg/L
128	179601-23-1	m,p-Xylene	3.38	mg/L
128	24959-67-9	Bromide	970	mg/L
128	71-43-2	Benzene	0.372	mg/L
128	7429-90-5	Aluminum	13.3	mg/L
128	7439-89-6	Iron	149	mg/L
128	7439-92-1	Lead	0.1	mg/L
128	7439-95-4	Magnesium	2260	mg/L
128	7439-96-5	Manganese	10.2	mg/L

SI Table 4a: 1198 chemicals reported as being detected in produced water, by reference

Refid	CAS	Name	Conc (Max reported)	Units
128	7440-23-5	Sodium	119000	mg/L
128	7440-24-6	Strontium	4660	mg/L
128	7440-29-1	Thorium	0.38	pCi/L
128	7440-39-3	Barium	2580	mg/L
128	7440-47-3	Chromium	0.14	mg/L
128	7440-66-6	Zinc	0.35	mg/L
128	74-82-8	Methane	10.5	mg/L
128	74-84-0	Ethane	2.73	mg/L
128	74-98-6	Propane	1.13	mg/L
128	7782-49-2	Selenium	0.34	mg/L
128	95-47-6	o-Xylene	0.673	mg/L
129	14808-79-8	Sulfate		
129	16887-00-6	Chloride		
129	7439-89-6	Iron		
129	7440-39-3	Barium		

SI Table 4b: Reference IDs

RefId	Citation
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SI Table 4b: Reference IDs

RefId	Citation
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SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
2157-01-9	Octyl methacrylate	Not Quantified								
2207-01-4	(Z)-1,2-Dimethylcyclohexane	Not Quantified			Yes					
2272-03-9	Butylidenecyclohexane	Not Quantified								
2274-11-5	Ethylene acrylate	Not Quantified			Yes					
2765-11-9	Pentadecanal	0.0453	mg/L							
2883-02-5	Cyclohexane, nonyl-	Not Quantified			Yes					
2883-05-8	Octane, 2-cyclohexyl-	Not Quantified								
2884-06-2	2,3-Dimethylnonane	Not Quantified								
2935-07-1	1H-Phenylene, dodecahydro-	Not Quantified								
4810-04-2	1,3,5-Trimethyl-2-propylbenzene	Not Quantified								
4810-09-7	3-Methyl-1-heptene	Not Quantified								
5161-04-6	Benzene, 1-methyl-4-(2-methylpropyl)-	Not Quantified			Yes					
5744-03-6	1H-Fluorene, dodecahydro-	Not Quantified								
5911-04-6	3-Methylnonane	Not Quantified			Yes					
7440-09-7	Potassium	66000	mg/L	Yes	Yes					Yes
7446-09-5	Sulfur dioxide	0.03225	mg/L	Yes	Yes					Yes
7783-06-4	Hydrogen sulfide	600	mg/L		Yes	Yes				Yes
100-01-6	4-Nitroaniline	0.0026	mg/L		Yes	Yes		Yes		Yes
10023-74-2	Pentanoic acid, ion(1-)	1.51689	mg/L							
1002-43-3	Undecane, 3-methyl-	Not Quantified								
1002-84-2	Pentadecanoic acid	0.00084	mg/L		Yes					
1003-64-1	Cyclohexane, ethylidene-	Not Quantified								
100-41-4	Ethylbenzene	4410	mg/L	Yes	Yes	Yes	Yes		Yes	Yes
100-42-5	Styrene	52	mg/L		Yes	Yes		Yes		Yes
10045-97-3	Caesium-137	9	pCi/L		Yes					Yes
100463-01-2	2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (cis)	Not Quantified								
100-49-2	Cyclohexanemethanol	Not Quantified			Yes					
100-51-6	Benzyl alcohol	0.34	mg/L		Yes	Yes				Yes
100-52-7	Benzaldehyde	Not Quantified		Yes	Yes	Yes				Yes
1008-80-6	2,3-Dimethyldecahydronaphthalene	Not Quantified								
10098-97-2	Strontium-90	70.7	pCi/L		Yes					Yes
1016165-79-9	1,2-Di-but-2-enyl-cyclohexane	0.00077	mg/L							
101-81-5	Diphenylmethane	0.00043	mg/L		Yes					
10198-40-0	Cobalt 60	Not Quantified			Yes					Yes
10222-95-4	5-Isopropyl-1,2,4-trimethylbenzene	Not Quantified								
1024-57-3	Heptachlor epoxide	Not Quantified			Yes	Yes	Yes	Yes	Yes	Yes
10317-17-6	Oxetane, 3-(1-methylethyl)-	Not Quantified								
103-40-2	Benzylsuccinate	0.006871029	mg/L							
103-65-1	Propylbenzene	1290	mg/L		Yes	Yes				Yes
10374-74-0	7-Tetradecene	Not Quantified								
10396-80-2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-ol	Not Quantified								
104-50-7	4-Octanolide	Not Quantified			Yes					
104-51-8	Butylbenzene	162	mg/L		Yes	Yes				Yes
104-61-0	gamma-Nonanolactone	Not Quantified			Yes					
104-76-7	2-Ethyl-1-hexanol	0.041	mg/L	Yes	Yes					Yes
10486-19-8	Tridecanal	0.0563	mg/L							
105-21-5	1,4-Heptanolide	Not Quantified			Yes					
10522-26-6	2-Methyl-1-undecanol	Not Quantified								
10544-50-0	Octasulfur	0.009629866	mg/L							
10544-95-3	Octadecane, 4-methyl-	Not Quantified								
105-60-2	Caprolactam	0.002392004	mg/L		Yes	Yes				Yes
105-67-9	2,4-Dimethylphenol	5	mg/L		Yes	Yes	Yes	Yes		Yes
105882-89-1	Ethanamine, 2,2'-azobis[N,N,1,1,2,2-hexafluoro-	Not Quantified								
10595-95-6	N-Nitroso-N-methylethylamine	Not Quantified			Yes	Yes		Yes		Yes
106-21-8	3,7-Dimethyloctan-1-ol	Not Quantified			Yes					

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
106-35-4	3-Heptanone	Not Quantified			Yes					
106-42-3	p-Xylene	0.46	mg/L		Yes				Yes	Yes
106-44-5	p-Cresol	0.3	mg/L		Yes	Yes				Yes
106-46-7	1,4-Dichlorobenzene	0.00034	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
106-51-4	1,4-Benzoquinone	0.00008	mg/L		Yes			Yes		Yes
106-65-0	Dimethyl succinate	0.8914662	mg/L	Yes	Yes					
106-90-1	Glycidyl acrylate	Not Quantified			Yes					
107-02-8	Acrolein	Not Quantified		Yes	Yes	Yes	Yes	Yes		Yes
107-13-1	Acrylonitrile	Not Quantified		Yes	Yes	Yes	Yes	Yes		Yes
1072-05-5	2,6-Dimethylheptane	Not Quantified			Yes					
107-21-1	Ethylene glycol	290	mg/L	Yes	Yes	Yes				Yes
1074-43-7	1-Methyl-3-propylbenzene	Not Quantified			Yes					
1075-06-5	Ethanone, 2,2-dihydroxy-1-phenyl-	Not Quantified								
1077-16-3	Benzene, hexyl-	Not Quantified								
107-83-5	2-Methylpentane	Not Quantified			Yes					
107-92-6	Butanoic acid	19	mg/L		Yes					
1079-71-6	1,2,3,4,5,6,7,8-Octahydroanthracene	0.00054	mg/L							
107997-59-1	1,2,3-Trimethyl-4-(3-methylbutyl)benzene	Not Quantified								
108-10-1	4-Methyl-2-pentanone	1.44	mg/L	Yes	Yes	Yes				Yes
1081-77-2	1-Phenylnonane	Not Quantified								
108-29-2	4-Pentanolide	Not Quantified			Yes					
108-38-3	m-Xylene	0.111	mg/L	Yes	Yes				Yes	Yes
108-39-4	m-Cresol	Not Quantified			Yes	Yes				Yes
108-67-8	1,3,5-Trimethylbenzene	6250	mg/L	Yes	Yes	Yes				Yes
108837-05-4	4-Propyl-9H-xanthen-9-one	0.00007	mg/L							
108-87-2	Methylcyclohexane	Not Quantified			Yes					Yes
108-88-3	Toluene	16800	mg/L	Yes	Yes	Yes	Yes	Yes	Yes	Yes
108-90-7	Chlorobenzene	0.35	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
108-91-8	Cyclohexylamine	0.034	mg/L		Yes	Yes				Yes
108-94-1	Cyclohexanone	Not Quantified			Yes	Yes				Yes
108-95-2	Phenol	6.96	mg/L	Yes	Yes	Yes		Yes		Yes
109-06-8	2-Methylpyridine	Not Quantified			Yes			Yes		Yes
109-21-7	Butyl butyrate	0.00044	mg/L		Yes					
109-52-4	Pentanoic acid	Not Quantified			Yes					
109-66-0	Pentane	Not Quantified		Yes	Yes	Yes				
109-74-0	Butanenitrile	Not Quantified			Yes					
110-27-0	Isopropyl tetradecanoic acid	0.00179	mg/L		Yes					
110-54-3	n-Hexane	Not Quantified		Yes	Yes	Yes				Yes
110-75-8	2-Chloroethyl vinyl ether	0.014	mg/L		Yes		Yes	Yes		Yes
110-82-7	Cyclohexane	5.97	mg/L		Yes	Yes				Yes
110-86-1	Pyridine	0.28	mg/L		Yes	Yes		Yes		Yes
110-94-1	Glutaric acid	0.290653	mg/L		Yes					
111-14-8	Heptanoic acid	0.3124488	mg/L		Yes					
111-16-0	Heptanedioic acid	0.1441521	mg/L		Yes					
111-27-3	1-Hexanol	Not Quantified			Yes					
111-30-8	Glutaraldehyde	Not Quantified		Yes	Yes	Yes				
111-44-4	Bis(2-chloroethyl) ether	Not Quantified		Yes	Yes	Yes	Yes	Yes		Yes
111-65-9	Octane	Not Quantified		Yes	Yes					
111-67-1	2-Octene	Not Quantified								
111-76-2	2-Butoxyethanol	77.5	mg/L	Yes	Yes	Yes				Yes
111-84-2	Nonane	Not Quantified		Yes	Yes	Yes				
1120-21-4	Undecane	0.0113	mg/L	Yes	Yes					
112-05-0	Nonanoic acid	Not Quantified			Yes					
112-18-5	N,N-Dimethyldodecan-1-amine	Not Quantified			Yes					
112-27-6	Triethylene glycol	17.8	mg/L	Yes	Yes	Yes				

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
112-30-1	1-Decanol	0.0054	mg/L	Yes	Yes					
1123-09-7	2-Cyclohexen-1-one, 3,5-dimethyl-	Not Quantified								
112-31-2	Decanal	Not Quantified			Yes					Yes
112-34-5	2-(2-Butoxyethoxy)ethanol	0.00045	mg/L	Yes	Yes	Yes				
112-37-8	Undecanoic acid	Not Quantified			Yes					
112-39-0	Methyl hexadecanoate	Not Quantified			Yes					
112-40-3	Dodecane	2.33	mg/L	Yes	Yes					Yes
112-41-4	1-Dodecene	Not Quantified		Yes	Yes					
1124-25-0	Cyclohexane, 1-methyl-4-(1-methylethenyl)-, trans-	Not Quantified								
1124-63-6	3-Cyclohexylpropan-1-ol	Not Quantified								
112-54-9	Dodecanal	0.0288	mg/L		Yes					
112-62-9	Methyl (9Z)-octadec-9-enoate	Not Quantified			Yes					
112-70-9	1-Tridecanol	Not Quantified			Yes					
112-75-4	N,N-Dimethyltetradecylamine	Not Quantified			Yes					
112-88-9	1-Octadecene	0.0463	mg/L	Yes	Yes					
112-89-0	1-Bromooctadecane	Not Quantified								
1129-29-9	1-Isopropenyl-3-isopropylbenzene	Not Quantified								
112-95-8	Eicosane	0.222	mg/L		Yes					Yes
1131-63-1	5,6,7,8-Tetrahydro-2-naphthoic acid	0.002995655	mg/L							
113-21-3	Lactate ion(1-)	Not Quantified			Yes					
1137-00-4	d,l-7-Azatriptophan	Not Quantified								
114482-57-4	4-Cyanophenyl 4-(3-butenyloxy)benzoate	Not Quantified								
114774-79-7	p-Nitrophenyl 1-azetidincarboxylate	Not Quantified								
115-22-0	2-Butanone, 3-hydroxy-3-methyl-	Not Quantified								
115-86-6	Triphenyl phosphate	0.00677137	mg/L		Yes					Yes
116164-06-8	3-Heptene, 2,2,3,5,6-pentamethyl-	Not Quantified								
116-53-0	2-Methylbutanoic acid	Not Quantified			Yes					
117-81-7	Di(2-ethylhexyl) phthalate	0.042	mg/L	Yes	Yes	Yes	Yes	Yes	Yes	Yes
117-84-0	Di-n-octyl phthalate	0.0093	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
118252-04-3	1-Hexyl-2-nitrocyclohexane	Not Quantified								
118-74-1	Hexachlorobenzene	0.001	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
118-90-1	2-Methylbenzoic acid	0.21784	mg/L		Yes					
1192-18-3	(Z)-1,2-Dimethylcyclopentane	Not Quantified								
119296-91-2	Methyl (4Z)-3,3-diphenylhex-4-enoate	0.002	mg/L							
1193-79-9	5-Methyl-2-furylmethylketone	Not Quantified								
119-61-9	Benzophenone	Not Quantified			Yes					Yes
119-64-2	Tetralin	0.00895	mg/L		Yes					
119-65-3	Isoquinoline	Not Quantified		Yes	Yes					Yes
119736-96-8	1',4-Dihydroxy-7'-methoxy-2,3'-dimethyl-,(-)-[1,2'-binaphthyl]	Not Quantified								
120-12-7	Anthracene	0.029	mg/L		Yes	Yes	Yes			Yes
1203-17-4	2,3-Dihydro-1,1,2,3,3-pentamethyl-1H-indene	0.00045	mg/L							
1205-39-6	2-Methyl-N-phenylaniline	0.00353	mg/L							
120-82-1	1,2,4-Trichlorobenzene	0.0015	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
120-83-2	2,4-Dichlorophenol	Not Quantified			Yes	Yes	Yes	Yes	Yes	Yes
121-33-5	4-Hydroxy-3-methoxybenzaldehyde	0.00431	mg/L		Yes					
121-91-5	1,3-Benzenedicarboxylic acid	0.3821036	mg/L		Yes					
122-20-3	Triisopropanolamine	Not Quantified		Yes	Yes					
122-39-4	Diphenylamine	0.00373	mg/L		Yes	Yes		Yes		Yes
122-66-7	1,2-Diphenylhydrazine	Not Quantified			Yes	Yes	Yes	Yes		Yes
122-84-9	2-Propanone, 1-(4-methoxyphenyl)-	Not Quantified			Yes					
123-05-7	2-Ethylhexanal	Not Quantified			Yes					
123-20-6	Butanoic acid, ethenyl ester	Not Quantified			Yes					
123-25-1	Diethyl butanedioate	1.4109876	mg/L		Yes					
123731-75-9	1-Allyl-3-methylindole-2-carbaldehyde	0.00149	mg/L							
123-79-5	Diocetyl hexanedioate	Not Quantified			Yes					

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
123-86-4	Butyl acetate	0.9	mg/L		Yes					Yes
123-91-1	1,4-Dioxane	0.06	mg/L	Yes	Yes	Yes		Yes		Yes
124-07-2	Octanoic acid	0.08220198	mg/L		Yes					
124-10-7	Methyl tetradecanoate	Not Quantified			Yes					
124-18-5	Decane	2.67	mg/L	Yes	Yes	Yes				Yes
1241-94-7	2-Ethylhexyl diphenyl phosphate	0.00075	mg/L		Yes					
124-25-4	Tetradecanal	0.0618	mg/L		Yes					
124-38-9	Carbon dioxide	634	mg/L	Yes	Yes					Yes
124-48-1	Chlorodibromomethane	Not Quantified			Yes	Yes	Yes		Yes	Yes
12587-46-1	Alpha particle	123000	pCi/L		Yes					Yes
12587-47-2	Beta particle	597600	pCi/L		Yes					Yes
12672-29-6	Aroclor 1248	Not Quantified			Yes	Yes	Yes		Yes	Yes
126-73-8	Tributyl phosphate	0.01896	mg/L	Yes	Yes	Yes				Yes
127-18-4	Tetrachloroethylene	0.005	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
128-39-2	2,6-Di-tert-butylphenol	Not Quantified			Yes					
129-00-0	Pyrene	0.23	mg/L		Yes	Yes	Yes			Yes
1300-71-6	Dimethylphenol	1.45	mg/L		Yes					
13066-95-0	1,3-Benzenediol, 4-amino-	Not Quantified								
131-11-3	Dimethyl phthalate	0.015	mg/L		Yes	Yes	Yes	Yes		Yes
13150-81-7	2,6-Dimethyldecane	Not Quantified								
13151-34-3	3-Methyldecane	Not Quantified			Yes					
13151-35-4	5-Methyldecane	Not Quantified								
13151-63-8	Cyclodecene, 1-methyl-, (E)-	Not Quantified								
13151-94-5	1,2-Dimethylcyclooctane	Not Quantified								
1319-77-3	Cresol	6.76	mg/L		Yes	Yes		Yes		
1321-94-4	Methylnaphthalene	0.015553579	mg/L		Yes					
13233-32-4	Radium-224	567.5675676	pCi/L							Yes
132-64-9	Dibenzofuran	0.0036	mg/L		Yes	Yes				Yes
132-65-0	Dibenzothiophene	0.0144	mg/L		Yes	Yes				Yes
13286-73-2	3-Ethyltridecane	Not Quantified								
13287-21-3	6-Methyltridecane	Not Quantified			Yes					
13287-23-5	8-Methylheptadecane	Not Quantified								
13287-24-6	9-Methylnonadecane	Not Quantified								
1330-20-7	Xylenes	11	mg/L	Yes	Yes	Yes			Yes	Yes
13432-25-2	3-hexanol, 2,4-dimethyl-	Not Quantified								
134-62-3	DEET	Not Quantified			Yes	Yes				Yes
13472-79-2	2-Hydroxy-5-iodopyridine	Not Quantified								
13485-66-0	2(1H)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-4a,8a-dimethyl-	Not Quantified								
13494-80-9	Tellurium	0.429	mg/L		Yes					Yes
135241-50-8	Propanamide, 2-(4-isobutylphenyl)-N-(3,5-dinitrophenyl)-	Not Quantified								
135-98-8	sec-Butylbenzene	270	mg/L		Yes	Yes				Yes
13632-94-5	1,4-Diethyl-2-methylbenzene	Not Quantified								
136-83-4	2-Nonylphenol	0.00791	mg/L							
13726-52-8	Diethyl N-(4-aminobenzoyl)-L-glutamate	Not Quantified								
13833-20-0	Amorphane	Not Quantified								
13925-05-8	Pyrazine, 2-methyl-5-(1-methylethyl)-	Not Quantified			Yes					
13943-77-6	Naphthalene, 1,2,3,4,4a,5,6,7-octahydro-4a-methyl-	Not Quantified								
13966-00-2	Potassium-40	700	pCi/L							Yes
13966-02-4	Beryllium-7	Not Quantified								
13966-29-5	Uranium 234	22.1	pCi/L		Yes					Yes
13967-63-0	Scandium-46	Not Quantified								
13981-52-7	Polonium-210	111.6216216	pCi/L							Yes
13982-63-3	Radium-226	16920	pCi/L		Yes				Yes	Yes
140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol	0.018338478	mg/L		Yes					Yes
14113-60-1	rel-(1R,2S)-1,2-Diethylcyclohexadecane	Not Quantified								

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
14123-41-2	3-Chloro-1,1,2,2-tetramethylcyclopropane	Not Quantified								
14127-61-8	Calcium ion	41000	mg/L		Yes					Yes
14158-27-1	Strontium-89	Not Quantified			Yes					Yes
142132-75-0	Propane, 1-(di-t-butylphosphino)-3-(2,4,6-tri-t-butylphenyl)	Not Quantified								
14250-88-5	2,2-Dimethylvaleraldehyde	Not Quantified								
14255-04-0	Lead-210	310	pCi/L		Yes					Yes
142-62-1	Hexanoic acid	0.766656	mg/L		Yes					Yes
14265-44-2	Phosphate	90	mg/L		Yes					Yes
14265-45-3	Sulfite	9.2	mg/L		Yes					Yes
14269-63-7	Thorium 230	9.37	pCi/L		Yes					
14274-82-9	Thorium 228	595.1351351	pCi/L		Yes					
14276-95-0	1H-Indene, 2,3-dihydro-1,1,6-trimethyl-	Not Quantified								
142-82-5	Heptane	Not Quantified		Yes	Yes	Yes				Yes
143-07-7	Dodecanoic acid	0.002517211	mg/L		Yes					
143-08-8	1-Nonanol	Not Quantified			Yes					
14331-83-0	Actinium 228	2054.054054	pCi/L		Yes					
14331-85-2	protactinium-231	240	pCi/L							
14339-23-2	1H-Pyrazole, 5-ethyl-4,5-dihydro-1,4-dimethyl-	Not Quantified								
14360-50-0	1-Hexanone, 1-(2-furanyl)-	Not Quantified			Yes					
14383-50-7	Thiosulfate	19.05989	mg/L							Yes
14398-67-5	Decalin, syn-1-methyl-, cis-	Not Quantified								
14398-71-1	cis-Decalin, 2-syn-methyl-	Not Quantified								
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	Not Quantified			Yes					
14449-42-4	1-sec-Butyladamantane	Not Quantified								
14451-87-7	Tricyclo(3.3.1.13.7)decane, 2-ethyl-	Not Quantified								
14451-88-8	2-n-Propyladamantane	Not Quantified								
1450-72-2	1-(2-Hydroxy-5-methylphenyl)ethanone	0.00029	mg/L							
1454-84-8	n-Nonadecanol-1	Not Quantified								
14676-29-0	3-Ethyl-2-methylheptane	Not Quantified			Yes					
1468-39-9	2-Methylbutanoic anhydride	Not Quantified								
146919-79-1	5-Methyl-1-undecene	Not Quantified								
14701-22-5	Nickel cation	19.2	mg/L							Yes
14733-03-0	Bismuth-214	7330	pCi/L							
14797-55-8	Nitrate	2670	mg/L		Yes	Yes			Yes	Yes
14797-65-0	Nitrite	219	mg/L		Yes	Yes			Yes	Yes
14798-03-9	Ammonium	1469	mg/L		Yes					Yes
14808-79-8	Sulfate	9164	mg/L		Yes					Yes
1483-60-9	2,4-Dimethyl-1-(1-methylpropyl)benzene	Not Quantified								
14859-67-7	Radon 222	139	pCi/L		Yes					
1486-75-5	cyclododecene, (e)-	Not Quantified								
14913-49-6	Bismuth-212	150	pCi/L							
14913-50-9	Thallium-208	0.4	pCi/L							
149-30-4	2-Mercaptobenzothiazole	0.00089	mg/L		Yes	Yes				Yes
14952-40-0	Actinium-227	2	pCi/L		Yes					
149-57-5	2-Ethylhexanoic acid	Not Quantified			Yes					
1502-38-1	Cyclooctane, methyl-	Not Quantified								
15035-72-0	Hydro sulfide	102.517	mg/L							
15065-10-8	Thorium 234	170	pCi/L		Yes					Yes
15067-28-4	Lead-214	7350	pCi/L							
15092-94-1	Lead-212	64.86486486	pCi/L							
15100-28-4	Protactinium-234	1400	pCi/L							
15117-96-1	Uranium-235	40	pCi/L		Yes					Yes
15123-40-7	Pyreno[4,5-c]furan	0.00183	mg/L							
1522-22-1	1,1,1,5,5,5-Hexafluoroacetylacetone	Not Quantified								
15229-37-5	Bismuth-211	2	pCi/L							

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15232-78-7	Cyclohexene,3-hexyl-	Not Quantified								
15232-85-6	Cyclohexene, 1-pentyl-	Not Quantified								
15232-86-7	1-Heptylcyclohexene	Not Quantified								
15262-20-1	Radium-228		3089 pCi/L		Yes				Yes	Yes
1528-22-9	Cyclobutane, (1-methylethylidene)-	Not Quantified								
15438-31-0	Fe +2 ion		656.72544 mg/L		Yes					Yes
15496-01-2	Ditrifluoromethyl(chlorocarbonyloxy)amine	Not Quantified								
1559-81-5	1-Methyltetraline		0.00069 mg/L							
1560-88-9	Octadecane, 2-methyl-	Not Quantified								
1560-89-0	Heptadecane, 2-methyl-	Not Quantified								
1560-92-5	2-Methylhexadecane	Not Quantified								
1560-93-6	2-Methylpentadecane	Not Quantified								
1560-95-8	2-Methyltetradecane	Not Quantified								
1560-96-9	2-Methyltridecane	Not Quantified								
1560-97-0	2-Methyldodecane		0.0097 mg/L							
15623-45-7	Radium-223		2 pCi/L							Yes
15623-47-9	Thorium 227		3 pCi/L		Yes					
156-60-5	(E)-1,2-Dichloroethylene		0.005 mg/L		Yes	Yes	Yes	Yes	Yes	Yes
1576-67-6	3,6-Dimethylphenanthrene		0.000334 mg/L							Yes
15869-86-0	4-Ethylcane	Not Quantified			Yes					
15869-93-9	3,5-Dimethyloctane	Not Quantified			Yes					
1595-10-4	1-Methyl-2-n-hexylbenzene	Not Quantified								
1595-16-0	1-(Butan-2-yl)-4-methylbenzene	Not Quantified								
1599-67-3	1-Docosene		0.00233 mg/L							
1606-08-2	Cyclopentylcyclohexane	Not Quantified								
16065-83-1	Chromium (III)		0.0447 mg/L		Yes	Yes				Yes
160951-15-5	4,6,8-Trimethyl-2-propylazulene		0.0004 mg/L							
1618-22-0	naphthalene, decahydro-2,6-dimethyl-	Not Quantified								
1620-98-0	3,5-Di-tert-butyl-4-hydroxybenzaldehyde		0.00042 mg/L							
1630-94-0	1,1-Dimethylcyclopropane	Not Quantified								
1632-70-8	Undecane, 5-methyl-	Not Quantified								
1636-44-8	Decane, 4-ethyl-	Not Quantified								
1640-89-7	Ethylcyclopentane	Not Quantified			Yes					
16538-89-9	cyclooctane, (1-methylpropyl)-	Not Quantified								
16580-24-8	1-Methyl-3-propan-2-ylcyclohexane	Not Quantified								
16580-26-0	cyclohexane, 1-isopropyl-1-methyl-	Not Quantified								
1660-04-4	Methyl tricyclo(3.3.1.1.3,7)dec-1-yl ketone	Not Quantified								
1667-00-1	Benzylcyclopropane	Not Quantified								
166773-56-4	2,3-Dimethyl-5-(2,6,10-trimethylundecyl) furan	Not Quantified								
16681-68-8	2H-1,2,3-Triazole-4-carbaldehyde	Not Quantified								
1671-77-8	1-Pentanone, 1-(4-methylphenyl)-	Not Quantified								
1674-10-8	Cyclohexene, 1,2-dimethyl-	Not Quantified			Yes					
16747-30-1	2,4,4-Trimethylhexane	Not Quantified			Yes					
16747-50-5	Cyclopentane, 1-ethyl-1- methyl-	Not Quantified								
1678-91-7	Ethylcyclohexane	Not Quantified			Yes					
1678-92-8	Propylcyclohexane	Not Quantified			Yes					
1678-93-9	Butylcyclohexane	Not Quantified			Yes					
1687-34-9	1-Ethyl-3-methyladamantane	Not Quantified								
1687-35-0	1,3-Dimethyl-5-ethyladamantane	Not Quantified								
1687-64-5	Phenol, 2-ethyl-6-methyl-	Not Quantified								
16887-00-6	Chloride		380000 mg/L	Yes	Yes					Yes
1689-64-1	Fluoren-9-ol		0.00032 mg/L		Yes					
16984-48-8	Fluoride		1100 mg/L		Yes				Yes	Yes
1703-51-1	2,5-Heptanedione	Not Quantified								
17059-48-2	1H-Indene, 2,3-dihydro-1,6-dimethyl-	Not Quantified								

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1718-52-1	Perdeuteriopyrene	0.0011	mg/L							
17301-23-4	2,6-Dimethylundecane	0.2018	mg/L							
17301-26-7	2,9-Dimethylundecane	Not Quantified								
17301-27-8	2,10-Dimethylundecane	Not Quantified								
17301-28-9	3,6-Dimethylundecane	Not Quantified			Yes					
17301-32-5	4,7-Dimethylundecane	Not Quantified								
17301-94-9	4-Methylnonane	Not Quantified			Yes					
17302-23-7	Nonane, 4,5-dimethyl-	Not Quantified								
17302-27-1	Nonane, 2,5-dimethyl-	Not Quantified								
17302-28-2	Nonane, 2,6-dimethyl-	Not Quantified								
17302-32-8	3,7-Dimethylnonane	Not Quantified								
17302-33-9	6-Methylundecane	Not Quantified								
1730-37-6	1-Methylfluorene	0.00051	mg/L							Yes
17312-50-4	2,5-Dimethyldecane	Not Quantified								
17312-53-7	3,6-Dimethyldecane	Not Quantified			Yes					
17312-54-8	3,7-Dimethyldecane	Not Quantified								
17312-55-9	3,8-Dimethyldecane	Not Quantified								
17312-57-1	3-Methyldodecane	0.0049	mg/L		Yes					
17312-59-3	Undecane, 4-ethyl-	Not Quantified								
17312-60-6	Undecane, 6-ethyl-	Not Quantified								
17312-62-8	5-Propyldecane	Not Quantified								
17312-77-5	2,3-Dimethylundecane	Not Quantified								
17312-80-0	2,4-Dimethylundecane	Not Quantified								
17312-81-1	3,5-Dimethylundecane	Not Quantified								
17341-25-2	Sodium ion	130000	mg/L							Yes
17429-36-6	2-Cyclohexen-1-one, 4-methyl-4-phenyl-	Not Quantified								
17453-94-0	Undecane, 5-ethyl-	Not Quantified								
1746-23-2	4-tert-Butylstyrene	Not Quantified			Yes					
1750-51-2	Naphthalene, decahydro-1,6-dimethyl-	Not Quantified								
1758-88-9	2-Ethyl-p-xylene	0.3469	mg/L		Yes					
176-63-6	Spiro(4-5)decane	Not Quantified								
1768-36-1	Propyl cyanate	Not Quantified								
17720-63-7	N,N,O-Triacetylhydroxylamine	Not Quantified								
17851-53-5	Butyl isobutyl phthalate	Not Quantified								
1786-12-5	1,7,11-Trimethyl-4-(1-methylethyl)cyclotetradecane	Not Quantified								
1795-15-9	Cyclohexane, octyl-	Not Quantified			Yes					
1795-16-0	Decylcyclohexane	Not Quantified			Yes					
179601-23-1	m,p-Xylene	46000	mg/L		Yes					Yes
180-43-8	Spiro(5.5)undecane	Not Quantified								
18294-04-7	Ethanedioic acid, bis(trimethylsilyl) ester	Not Quantified								
18344-37-1	heptadecane, 2,6,10,14-tetramethyl-	Not Quantified								
1839-63-0	1,3,5-Trimethylcyclohexane	Not Quantified			Yes					
18420-41-2	2-(Chloromethyl)tetrahydropyran	Not Quantified								
18435-22-8	Tetradecane, 3-methyl-	Not Quantified								
18435-45-5	1-Nonadecene	0.00215	mg/L							
18496-25-8	Sulfide	7700	mg/L		Yes					Yes
1849-76-9	3-bromo-5-chloro-4-hydroxybenzaldehyde	Not Quantified								
18540-29-9	Chromium (VI) ion	5.4	mg/L		Yes	Yes				Yes
1871-67-6	2-Octenoic acid	Not Quantified								
1879-07-8	Cyclohexane, 1-methyl-4-(1-methylethenyl)-, cis-	Not Quantified								
18835-32-0	1-Tricosene	Not Quantified								
18835-33-1	1-Hexacosene	0.00204	mg/L							
188645-81-0	3,4-Dichlorophenol, tert-butyl(dimethylsilyl) ether	Not Quantified								
1888-57-9	3-Hexanone, 2,5-dimethyl- (8Cl)(9Cl)	Not Quantified								
191-24-2	Benzo(g,h,i)perylene	0.0015	mg/L		Yes		Yes			Yes

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1921-70-6	Norphytane	0.0952	mg/L							
19218-94-1	1-Iodotetradecane	Not Quantified								
19219-84-2	benzene, (1,3-dimethylbutyl)-	Not Quantified								
19261-13-3	1-(2-Furanyl)-3-butene-1,2-diol	Not Quantified								
193-39-5	Indeno(1,2,3-cd)pyrene	0.022	mg/L		Yes	Yes	Yes	Yes		Yes
19385-87-6	1,3-Dimethyl-5-n-propyl-adamantane	Not Quantified								
19549-87-2	2,4-Dimethyl-1-heptene	Not Quantified								
19550-75-5	2,2-dimethyl-3-heptene trans	Not Quantified								
19744-64-0	1H-Indene, octahydro-5-methyl-	Not Quantified								
19781-34-1	3-ethyl-3-phenyl-1-pentene	Not Quantified								
19781-86-3	8-Hexadecyne	0.00028	mg/L							
198-55-0	Perylene	Not Quantified			Yes					Yes
1985-59-7	1,1-Dimethyl(1,2,3,4-tetrahydronaphthalene)	Not Quantified								
1985-88-2	4-Chloro-2-methyl-2-butanol	Not Quantified								
1985-97-3	(3-methylpentan-3-yl)benzene	Not Quantified								
2027-17-0	2-Isopropyl-naphthalene	Not Quantified								Yes
20278-89-1	Heptane, 3,4,5-trimethyl-	Not Quantified								
20291-73-0	Dimethylphenanthrene	0.00149	mg/L							
20309-77-7	Cyclopentane, 1,1,3,4-tetramethyl-, trans-	Not Quantified								
20396-49-0	tert-Butyl cyclohexanecarboxyperoxyate	Not Quantified								
2040-96-2	Propylcyclopentane	Not Quantified			Yes					
204781-73-7	28-Nor-17alpha(H)-hopane	0.00126	mg/L							
2049-95-8	tert-Pentylbenzene	Not Quantified			Yes					
2051-30-1	2,6-Dimethyloctane	Not Quantified			Yes					
20524-86-1	Bis(dichloromethyl) ether	Not Quantified								
205-82-3	Benzo(j)fluoranthene	Not Quantified			Yes	Yes		Yes		Yes
205-99-2	Benzo(b)fluoranthene	0.006	mg/L		Yes	Yes	Yes	Yes		Yes
20633-03-8	2,2,5-Trimethylhexane-3,4-dione	Not Quantified								
206-44-0	Fluoranthene	0.035	mg/L		Yes	Yes	Yes	Yes		Yes
207-08-9	Benzo(k)fluoranthene	0.0049	mg/L		Yes	Yes		Yes		Yes
2082-59-9	valeric anhydride	Not Quantified								
208-96-8	Acenaphthylene	0.11	mg/L		Yes		Yes			Yes
20959-33-5	Heptadecane, 7-methyl-	Not Quantified								
2103-57-3	2,3,4-Trimethoxybenzaldehyde	0.00039	mg/L							
21195-59-5	1,5,8-p-Menthatriene	Not Quantified								
2131-41-1	1,4,5-Trimethylnaphthalene	Not Quantified								
2131-42-2	1,4,6-Trimethylnaphthalene	Not Quantified								
21524-26-5	Cyclohexene, 4-butyl-	Not Quantified								
21693-54-9	5,7-Dimethyltetralin	Not Quantified								
21693-55-0	1,5,7-Trimethyl-1,2,3,4-tetrahydronaphthalene	Not Quantified								
218-01-9	Chrysene	0.11	mg/L		Yes	Yes	Yes	Yes		Yes
21868-43-9	s-Triazine, 2-amino-4-(piperidinomethyl)-4-piperidino-	Not Quantified								
2189-60-8	Benzene, octyl-	Not Quantified								
219783-06-9	1-Isopropyl-1,4,5-trimethylcyclohexane	Not Quantified								
22052-84-2	Heptafluoroisopropyl methyl ether	Not Quantified								
22089-89-0	7-pentadecyne	Not Quantified								
2213-23-2	2,4-Dimethylheptane	Not Quantified			Yes					
2216-33-3	3-Methyloctane	Not Quantified			Yes					
2216-34-4	4-Methyloctane	Not Quantified			Yes					
2234-20-0	2,4-Dimethylstyrene	Not Quantified								
2234-75-5	1,2,4-Trimethylcyclohexane	Not Quantified								
2245-38-7	1,6,7-Trimethylnaphthalene	Not Quantified			Yes					Yes
22531-20-0	6-Ethyl-1,2,3,4-tetrahydronaphthalene	Not Quantified								
22537-38-8	Rubidium, ion (Rb1+)	0.038	mg/L							
227327-87-9	N-Adamantan-1-ylmethyl-2-chloro-5-nitro-benzamide	Not Quantified								

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228729-94-0	8,13-Dimethyl-14-(3-methylbutyl)podocarpene	0.00175	mg/L							
2292-79-7	Congressane	Not Quantified								
2294-72-6	5-Undecyne	Not Quantified								
23051-84-5	5-Tridecene, (5E)-	Not Quantified				Yes				
2315-61-9	2-[2-[4-(1,1,3,3-Tetramethylbutyl)phenoxy]ethoxy]ethanol	0.00134	mg/L		Yes					
23183-11-1	1,1'-Bicycloheptyl	Not Quantified								
23342-25-8	2,2,5,7-Tetramethyltetralin	Not Quantified								
23609-46-3	cyclooctane, 1,2-diethyl-	Not Quantified								
2363-88-4	2,4-Decadienal	Not Quantified								
2381-21-7	1-Methylpyrene	0.0000477	mg/L		Yes					Yes
2385-77-5	(3R)-3,7-Dimethyloct-6-enal	Not Quantified								
2399-48-6	Tetrahydrofurfuryl acrylate	Not Quantified								
2406-25-9	Di-tert-butyl nitroxide	Not Quantified								
24145-88-8	(E)-1,4-Dimethyladamantane	Not Quantified								
24145-89-9	(Z)-1,4-Dimethyladamantane	Not Quantified								
2416-20-8	hexadecenoic acid, z-11-	Not Quantified								
243-38-9	5H-Quinindoline	Not Quantified								
2435-85-0	Hexadecahydropyrene	Not Quantified								
2437-56-1	1-Tridecene	Not Quantified			Yes					
2440-22-4	2-(2H-Benzotriazol-2-yl)-4-methylphenol	0.00091	mg/L		Yes					
24451-17-0	ethyl 2-(3,4-dimethylanilino)-2-oxoacetate	Not Quantified								
2453-00-1	1,3-Dimethylcyclopentane	Not Quantified			Yes					
24624-29-1	1-Ethyl-9,10-anthraquinone	0.00012	mg/L							
2471-83-2	1-Ethylidene-1H-indene	Not Quantified								
2471-84-3	1-Methylene-1H-indene	Not Quantified								
24959-67-9	Bromide	13600	mg/L		Yes					Yes
2499-95-8	Hexyl acrylate	Not Quantified			Yes					
25117-24-2	4-Methyltetradecane	Not Quantified								
25117-31-1	5-Methyltridecane	Not Quantified								
25117-32-2	5-Methyltetradecane	Not Quantified								
25117-35-5	Octadecane, 5-methyl-	Not Quantified								
25167-82-2	Trichlorophenol	Not Quantified			Yes					Yes
25167-94-6	Diphenylpropane	0.00022	mg/L							
25201-40-5	1,6-Heptadien-4-ol, 4-methyl-	Not Quantified								
2531-84-2	2-Methylphenanthrene	Not Quantified								
25322-68-3	Polyethylene glycol	16	mg/L	Yes	Yes					Yes
25322-69-4	Polypropylene glycol	Not Quantified		Yes	Yes					Yes
25377-73-5	3-(Dodecenyldihydro-2,5-furandione	0.00116	mg/L		Yes					
25414-22-6	2-Methoxyfuran	Not Quantified								
25415-84-3	Butanoic acid, 2-ethylhexyl ester	0.0004	mg/L							
2541-75-5	8-heptadecanol	Not Quantified								
25419-33-4	naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	Not Quantified								
25447-95-4	Hexadecenoic acid	0.008368372	mg/L							
2547-26-4	4a-Methyldecalin	Not Quantified								
25524-42-9	5-Tridecene, (Z)-	Not Quantified								
25551-13-7	Trimethylbenzene	Not Quantified		Yes	Yes					Yes
2566-97-4	9,12-octadecadienoic acid, methyl ester, (e,e)-	Not Quantified								
25711-30-2	1H-Pyrazole-4-carboxaldehyde, 1,5-dimethyl-	Not Quantified								
26321-98-2	Cyclohexane, (1-ethylpropyl)-	Not Quantified								
26429-11-8	4-Methylheptadecane	Not Quantified								
2658-24-4	2,2-Dimethylaziridine	0.0002	mg/L							
26603-23-6	Bis(octylphenyl)amine	0.00019	mg/L							
26730-12-1	4-Methyltridecane	Not Quantified								
26730-14-3	7-Methyltridecane	Not Quantified								
26730-20-1	7-Methylhexadecane	Not Quantified								

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
26746-38-3	2,3-di-tert-butylphenol	Not Quantified								
26761-40-0	Diisodecyl phthalate	Not Quantified			Yes					
26764-26-1	Octadecenoic acid	0.003472104	mg/L							
2682-20-4	2-Methyl-3(2H)-isothiazolone	9.51	mg/L	Yes	Yes					
268543-19-7	1-Ethanone, 1-(1-adamantyl)-2-phenyl-	Not Quantified								
26967-64-6	Cyclohexane, (1-methylpropyl)-	Not Quantified								
2717-39-7	1,4,5,8-Tetramethylnaphthalene	Not Quantified								
272-16-2	1,2-Benzisothiazole	Not Quantified								
274691-67-7	Dithiocarbaminic acid, N-cyano-, S-[3-(4-ethylphenyl)-3-oxo-	Not Quantified								
27519-02-4	(Z)-9-Tricosene	0.00098	mg/L		Yes					
27530-79-6	Simonellite	0.00068	mg/L							
27554-26-3	Diisooctyl phthalate	Not Quantified			Yes					
27601-00-9	Methylquinoline	0.003749272	mg/L							
276890-11-0	5-(1,1-Dimethylethyl)-1H-indene	0.0001	mg/L							
27875-89-4	1-Phenanthrenecarboxylic acid	0.00012	mg/L							
28071-99-0	trans-anti-trans-tetra-decahydroanthracene	Not Quantified								
2809-64-5	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	Not Quantified								
281-23-2	Adamantane	74	mg/L		Yes					
2815-57-8	1,2,3-Trimethylcyclopentane	Not Quantified								
2815-58-9	1,2,4-Trimethylcyclopentane	Not Quantified			Yes					
2847-72-5	4-Methyldecane	Not Quantified			Yes					
2855-19-8	1,2-Epoxydodecane	Not Quantified			Yes					
286-20-4	Cyclohexene oxide	Not Quantified			Yes					
28652-72-4	Methyl-1,1'-biphenyl	0.00213067	mg/L							
286-63-5	9-Thiabicyclo[6.1.0]nonane	Not Quantified								
28804-88-8	Dimethylnaphthalene	0.009506014	mg/L		Yes					
2882-96-4	pentadecane, 3-methyl-	Not Quantified			Yes					
2882-98-6	n-Nonylcyclopentane	Not Quantified								
2885-00-9	1-Octadecanethiol	Not Quantified								
2896-60-8	4-Ethylresorcinol	Not Quantified								
28980-74-7	3,5-Dodecadiene, 2-methyl-	Not Quantified								
28981-49-9	Ethylcyclododecane	0.00154	mg/L							
29053-04-1	Cyclopentane, 1-methyl-3-(2-methylpropyl)-	Not Quantified								
294-62-2	Cyclododecane	Not Quantified			Yes					
295-02-3	Cyclotridecane	Not Quantified								
295-17-0	Cyclotetradecane	Not Quantified								
295-48-7	Cyclopentadecane	Not Quantified								
2958-76-1	Decahydro-2-methylnaphthalene	Not Quantified								
296-56-0	Cycloeicosane	Not Quantified								
297-35-8	Cyclotriacontane	0.00108	mg/L							
29799-19-7	Cyclohexane, 1-(1,5-dimethylhexyl)-4-methyl-	Not Quantified								
298-02-2	Phorate	Not Quantified			Yes	Yes		Yes		Yes
2980-69-0	4-Methylundecane	Not Quantified								
30159-17-2	Tricyclo[7.3.0.0(2,6)]dodecane, trans-anti-trans-	Not Quantified								
30232-26-9	Trimethylphenanthrene	0.00012	mg/L		Yes					
3031-15-0	1,2,3,4-Tetramethylnaphthalene	Not Quantified								
30316-17-7	1,2,3,4-Tetrahydro-2,5,8-trimethylnaphthalene	Not Quantified								
3055-93-4	2-[2-(Dodecyloxy)ethoxy]ethanol	Not Quantified								
3055-94-5	Triethylene glycol monododecyl ether	Not Quantified								
30654-45-6	Naphthalene, 6-butyl-1,2,3,4-tetrahydro-	Not Quantified								
30677-34-0	Cyclohexane, ethylmethyl-	Not Quantified								
3073-66-3	1,1,3-Trimethylcyclohexane	Not Quantified			Yes					
3074-71-3	2,3-Dimethylheptane	Not Quantified			Yes					
307-55-1	Perfluorododecanoic acid	Not Quantified			Yes					Yes
309-00-2	Aldrin	Not Quantified			Yes	Yes	Yes	Yes		Yes

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
309735-29-3	1,2-Benzisothiazole, 3-(hexahydro-1H-azepin-1-yl)-, 1,1-di	0.00066	mg/L							
31061-61-7	Tricyclo[4.3.1.1(3,8)]undecane-3-carboxylic acid, methyl e	Not Quantified								
31295-56-4	2,6,11-Trimethyldodecane	Not Quantified								
3147-55-5	Benzoic acid, 3,5-dibromo-2-hydroxy-	Not Quantified								
315244-85-0	Pyrazolo[3,4-b]pyran-5-carbonitrile, 1,4-dihydro-6-amino-4	Not Quantified								
3178-23-2	Dicyclohexylmethane	Not Quantified								
319-85-7	beta-Hexachlorocyclohexane	Not Quantified			Yes	Yes	Yes			Yes
319-86-8	delta-Hexachlorocyclohexane	0.00048	mg/L		Yes		Yes			Yes
32038-83-8	2-Propynenitrile, 3-fluoro-	0.00018	mg/L							
3221-61-2	2-Methyloctane	Not Quantified			Yes					
32367-54-7	Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-	Not Quantified								
3282-53-9	Cyclohexene, 1-butyl-	Not Quantified								
331835-05-3	1-(2,4-Dihydroxybenzoyl)-3-ethyl-5-trifluoromethyl-5-hydro	Not Quantified								
33213-65-9	Endosulfan II	Not Quantified			Yes					Yes
3333-52-6	Tetramethylsuccinonitrile	Not Quantified			Yes					
334-48-5	Decanoic acid	Not Quantified			Yes					
337503-48-7	4-Pentenoic acid, 2,2-diethyl-3-oxo-5-phenyl-, ethyl ester	Not Quantified								
3386-33-2	Octadecyl chloride	0.00212	mg/L		Yes					
33933-74-3	3-Heptene, 4-ethyl-	Not Quantified								
3404-73-7	1-Pentene, 3,3-dimethyl-	Not Quantified			Yes					
3430-33-9	2,6-Dimethyl-3-pyridylamine	Not Quantified								
34303-81-6	3-Hexadecene, (Z)-	Not Quantified								
343270-50-8	2-(Butyliden-2-one)tetrahydrofuran	Not Quantified								
34694-70-7	1,3,5,6-Tetramethyladamantane	Not Quantified								
35216-11-6	7-Tetradecyne	0.00038	mg/L							
352-70-5	m-Fluorotoluene	Not Quantified			Yes					
35354-38-2	7-Octadecyne, 2-methyl-	Not Quantified								
35365-59-4	9-Octadecyne	Not Quantified								
36947-68-9	1H-Imidazole, 2-(1-methylethyl)-	Not Quantified								
371-40-4	4-Fluoroaniline	Not Quantified			Yes					
3726-46-3	1-Ethyl-2-methylcyclopentane	Not Quantified								
3728-54-9	1-Ethyl-2-methylcyclohexane	Not Quantified								
3728-55-0	1-Ethyl-3-methylcyclohexane	Not Quantified								
3728-56-1	1-Ethyl-4-methylcyclohexane	Not Quantified			Yes					
376-77-2	Decafluorocyclopentane	Not Quantified								
3777-69-3	2-Pentylfuran	Not Quantified			Yes					
3777-70-6	2-Hexylfuran	Not Quantified								
3777-71-7	Furan, 2-heptyl-	Not Quantified			Yes					
3812-32-6	Carbonate	17000	mg/L		Yes					Yes
38274-72-5	(Z)-4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane	Not Quantified								
38489-80-4	Benzaldehyde, 3-methoxy-, oxime	Not Quantified								
3877-19-8	Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	Not Quantified								
3891-98-3	2,6,10-Trimethyldodecane	0.00096	mg/L		Yes					
3892-00-0	2,6,10-Trimethylpentadecane	Not Quantified								
39178-69-3	3-butylcyclohexanone	Not Quantified								
39546-79-7	Pentylidenecyclohexane	Not Quantified								
4013-34-7	(1-Methoxyethyl)benzene	Not Quantified								
4032-93-3	heptane, 2,3,6-trimethyl-	Not Quantified			Yes					
40650-41-7	1,1,5-Trimethylindan	Not Quantified								
40710-32-5	Nonahexacontanoic acid	Not Quantified								
4132-72-3	Benzene, 1,4-dimethyl-2-(1-methylethyl)-	Not Quantified								
41446-57-5	3-Tridecene, (3E)-	Not Quantified								
41446-59-7	2-tridecene, (z)-	Not Quantified								
41446-60-0	7-Tetradecene, (Z)-	Not Quantified								
41446-65-5	4-Tetradecene, (Z)-	Not Quantified								

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
41446-66-6	5-tetradecene, (e)-	Not Quantified			Yes					
41446-68-8	3-Tetradecene, (E)-	Not Quantified								
41446-78-0	4-Tetradecene, (4E)-	Not Quantified								
4175-53-5	1H-Indene, 2,3-dihydro-1,3-dimethyl-	Not Quantified								
4175-54-6	Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	Not Quantified								
41977-45-1	Bicyclo[4.1.0]heptane, 7-pentyl-	Not Quantified								
41977-48-4	bicyclo[4.1.0]heptane, 3-methyl-7-pentyl-	Not Quantified								
4218-48-8	Benzene, 1-ethyl-4-(1-methylethyl)-	Not Quantified								
4237-46-1	Benzoyldiphenylmethanol	Not Quantified								
42775-75-7	naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	Not Quantified								
42775-77-9	6-n-Propyltetralin	Not Quantified								
4282-44-4	Undecane, 1-iodo-	Not Quantified								
4291-79-6	1-Methyl-2-propyl-cyclohexane	Not Quantified								
4292-75-5	Hexylcyclohexane	Not Quantified			Yes					
4292-92-6	Pentylcyclohexane	Not Quantified			Yes					
4306-65-4	1,1,3,5-Tetramethylcyclohexane	Not Quantified								
432-04-2	Phosphine, tris(trifluoromethyl)-	Not Quantified								
4359-46-0	1,3-Dioxolane, 2-ethyl-4-methyl-	Not Quantified								
4360-57-0	2-Pentadecyl-1,3-dioxolane	Not Quantified								
4413-16-5	Benzene, (1-cyclohexylethyl)-	Not Quantified								
4413-21-2	1,1-Dicyclopentylethane	Not Quantified								
442662-72-8	2-Ethyl-1,1,3-trimethylcyclohexane	Not Quantified								
4431-89-4	(Cyclopentylmethyl)cyclohexane	Not Quantified								
4453-90-1	1,4-Dihydro-1,4-methanonaphthalene	Not Quantified								
4457-00-5	Cyclopentane, hexyl-	Not Quantified								
4461-48-7	4-Methyl-2-pentene	Not Quantified								
4466-77-7	1,2,3,4-Tetramethylphenanthrene	0.00068 mg/L								
4516-69-2	1,1,3-Trimethylcyclopentane	Not Quantified			Yes					
4551-51-3	1H-Indene, octahydro-, cis-	Not Quantified								
461-55-2	Butyrate		3 mg/L							
4674-23-1	1,2-Di(2,4,6-trimethylphenyl)ethane	Not Quantified								
4701-36-4	Benzene, (1-ethyl-1-propenyl)-	Not Quantified								
4706-90-5	1,3-Dimethyl-5-isopropylbenzene	Not Quantified								
471-34-1	Carbonic acid calcium salt (1:1)		103026 mg/L	Yes	Yes					Yes
47145-46-0	3,4-Dihydroisouquinolin-7-ol, 1-[4-hydroxybenzyl]-6-methoxy-	Not Quantified								
475-03-6	1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene	Not Quantified								
480-72-8	Acenaphthylene, 1,2,2a,3,4,5-hexahydro-	Not Quantified								
48134-26-5	2,4,6-Trimethylazulene	0.00049 mg/L								
483-65-8	Retene	0.00319 mg/L			Yes					
483-78-3	Cadalene	0.00032 mg/L								
489-20-3	1-Isopropyl-2,3-dimethylcyclopentane	Not Quantified								
490-65-3	1-Methyl-7-isopropyl-naphthalene	Not Quantified								
4912-92-9	1,1-Dimethylindan	Not Quantified								
4920-99-4	Benzene, 1-ethyl-3-(1-methylethyl)-	Not Quantified								
493-02-7	Naphthalene, decahydro-, trans-	Not Quantified			Yes					
4957-14-6	1-Methyl-4-[(4-methylphenyl)methyl]benzene	0.00011 mg/L			Yes					
496-11-7	Indan	0.0096 mg/L			Yes					
497-32-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-5-methylene-	Not Quantified								
50-00-0	Formaldehyde	0.8 mg/L	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
5004-45-5	4-Phenylphthalazin-1(2H)-one	Not Quantified								
50-24-8	Prednisolone	0.00051 mg/L			Yes					Yes
50-32-8	Benzo(a)pyrene	0.035 mg/L			Yes	Yes	Yes	Yes	Yes	Yes
503-74-2	Isovaleric acid	0.96 mg/L			Yes					
50617-19-1	2,5,8-Triphenyl benzotriazole	Not Quantified								
506-43-4	(Z,Z)-9,12-Octadecadien-1-ol	Not Quantified								

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
50876-32-9	CYCLOHEXANE, 1,1,3,5-TETRAMETHYL-, CIS-	Not Quantified								
50991-08-7	1,1'-Bicyclohexyl, 2-methyl-, cis-	Not Quantified								
50991-09-8	1,1'-Bicyclohexyl, 2-methyl-, trans-	Not Quantified								
50991-12-3	1,1'-Bicyclohexyl, 2-ethyl-, cis-	Not Quantified								
50991-13-4	1,1'-Bicyclohexyl, 2-ethyl-, trans-	Not Quantified								
51050-50-1	2-Methyl-7-octadecene	Not Quantified								
513-35-9	2-Methyl-2-butene	Not Quantified			Yes					
526-73-8	1,2,3-Trimethylbenzene	Not Quantified		Yes	Yes	Yes				Yes
527-54-8	3,4,5-Trimethylphenol	Not Quantified								
52845-07-5	Isoeicosane	0.00258	mg/L							
52856-01-6	2-Ethoxy-4,4,5,5-tetramethyloxazoline	Not Quantified								
52873-50-4	1,3-Dimethyl-5-n-hexyladamantane	Not Quantified								
52896-87-4	Heptane, 4-(1-methylethyl)-	Not Quantified								
52914-66-6	Cyclopentadecanone, 2-methyl-	Not Quantified								
529-34-0	1,2,3,4-Tetrahydronaphthalen-1-one	Not Quantified			Yes					
53172-84-2	(1-Methyl-1-buten-1-yl)benzene	Not Quantified								
533-18-6	Acetic acid, 2-methylphenyl ester	0.05556549	mg/L		Yes					
53366-55-5	Pentylidenecyclopentane	Not Quantified								
5337-61-1	2-Octadecyl-1,3-propanediol	0.00042	mg/L							
53485-49-7	Tricyclo[6.4.0.0(2,7)]dodecane	Not Quantified								
53535-33-4	Heptanol	Not Quantified								
535-77-3	m-Cymene	Not Quantified			Yes					
53-70-3	Dibenz(a,h)anthracene	0.023	mg/L		Yes	Yes	Yes	Yes		Yes
53715-09-6	Chloro(iodo)acetic acid	Not Quantified								
5380-87-0	Furfuryl glycidyl ether	Not Quantified								
538-68-1	Pentylbenzene	Not Quantified			Yes					
538-86-3	Benzyl methyl ether	Not Quantified			Yes					
53907-60-1	Cyclopentane, 1,1,3,4-tetramethyl-, cis-	Not Quantified								
5402-53-9	Chloromethyl propanoate	Not Quantified								
54105-66-7	Undecylcyclohexane	Not Quantified								
54105-77-0	(2-methylbutyl)cyclohexane	Not Quantified								
54163-69-8	Isopilocarpine	Not Quantified								
541-73-1	1,3-Dichlorobenzene	0.0003	mg/L		Yes	Yes	Yes	Yes		Yes
541-91-3	3-Methylcyclopentadecan-1-one	Not Quantified			Yes					
542-28-9	Tetrahydro-2H-pyran-2-one	Not Quantified			Yes					
54290-12-9	7-heptadecene	Not Quantified								
54410-74-1	1-Methyl-2-(1-ethylpropyl)benzene	Not Quantified								
54410-98-9	1-nonene, 4,6,8-trimethyl-	Not Quantified								
54411-00-6	cyclohexane, 1-methyl-4-(1-methylbutyl)-	Not Quantified								
54411-01-7	1-Methyl-2-pentylcyclohexane	Not Quantified								
54411-17-5	Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1à,2à,4à)	Not Quantified								
544-25-2	1,3,5-Cycloheptatriene	Not Quantified			Yes					
544-63-8	Tetradecanoic acid	0.005315497	mg/L		Yes					
544-76-3	Hexadecane	0.601	mg/L	Yes	Yes					Yes
544-85-4	Dotriacontane	Not Quantified								
5466-77-3	Octinoxate	0.00278	mg/L		Yes					
54676-39-0	2-BUTYL-1,1,3-TRIMETHYL-CYCLOHEXANE	Not Quantified								
54699-35-3	1,2,4-Benzenetricarboxylic acid, 1,2-dimethyl ester	Not Quantified								
54766-91-5	Bicyclo[10.1.0]tridec-1-ene	Not Quantified								
54823-95-9	Cyclohexane, 1-(cyclohexylmethyl)-3-methyl-, trans-	Not Quantified								
54823-97-1	cis-1-(Cyclohexylmethyl)-4-methylcyclohexane	Not Quantified								
54823-98-2	Cyclohexane, 1-(cyclohexylmethyl)-4-methyl-, trans-	Not Quantified								
54827-17-7	3,3',5,5'-Tetramethylbenzidine	Not Quantified			Yes					
54832-83-6	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	Not Quantified								
54833-23-7	10-Methylcosane	Not Quantified								

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
54833-48-6	Heptadecane, 2,6,10,15-tetramethyl	Not Quantified								
54965-05-8	Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-	Not Quantified								
55030-62-1	Tridecane, 4,8-dimethyl-	Not Quantified								
55044-33-2	1h-indene, 2-butyl-5-hexyloctahydro-	Not Quantified								
55045-07-3	2-Methyl-8-propyldodecane	0.00052	mg/L							
55170-90-6	Bicyclo[2.2.1]heptane, 2-(1-buten-3-yl)-	Not Quantified								
55282-11-6	11-Pentan-3-ylhenicosane	Not Quantified								
55282-34-3	Cyclohexane, 1,3,5-trimethyl-2-octadecyl-	Not Quantified								
55282-68-3	2-Dodecyl- 1,1':3',1"-tercyclopentane	Not Quantified								
55402-13-6	2,2,7-Trimethyl-3-octyne	Not Quantified								
554-59-6	Carane	Not Quantified								
5557-93-7	Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-	Not Quantified								
556-67-2	Octamethylcyclotetrasiloxane	Not Quantified		Yes	Yes					Yes
55669-88-0	1-Isobutyl-2,5-dimethylbenzene	Not Quantified								
55682-81-0	3-tert-Butyl-1,2-dihydronaphthalene	Not Quantified								
557-35-7	octane, 2-bromo-	Not Quantified								
5579-66-8	3,6,9,12,15,18,21,24,27-Nonaoxanonacosane-1,29-diol	Not Quantified								
55821-04-0	syn-1,6:8,13-Bismethano[14]annulene	Not Quantified								
56009-20-2	1-(1,5-Dimethylhexyl)-4-(4-methylpentyl)cyclohexane	Not Quantified								
5618-62-2	O-Isobutylhydroxylamine	Not Quantified								
56221-91-1	13-Tetradecen-1-yl acetate	Not Quantified								
562-28-7	(-)-Kaur-16-ene	0.00136	mg/L		Yes					
56292-65-0	2,5-Dimethyldodecane	Not Quantified								
56292-69-4	Tetradecane, 2,5-dimethyl-	Not Quantified								
563-16-6	3,3-Dimethylhexane	Not Quantified			Yes					
56325-56-5	Cyclodecene, 3-bromo-	Not Quantified								
563-46-2	2-Methylbut-1-ene	Not Quantified			Yes					
56442-17-2	4-(4-Fluorobenzoyloxy)benzaldehyde	Not Quantified								
56-55-3	Benz(a)anthracene	0.017	mg/L		Yes	Yes	Yes	Yes		Yes
565-67-3	3-Pentanol, 2-methyl-	Not Quantified								
5661-80-3	Bicyclo[5.3.0]decane	Not Quantified								
56936-67-5	Glycine, N-trifluoroacetyl-, isopropyl ester	Not Quantified								
57-10-3	Hexadecanoic acid	0.003021193	mg/L		Yes					
57-11-4	Octadecanoic acid	0.00373392	mg/L		Yes					
57-12-5	Cyanide	3	mg/L		Yes	Yes	Yes		Yes	Yes
571-58-4	1,4-Dimethylnaphthalene	Not Quantified			Yes					
571-61-9	1,5-Dimethylnaphthalene	Not Quantified			Yes					
5743-97-5	phenanthrene, tetradecahydro-	Not Quantified								
575-43-9	1,6-Dimethylnaphthalene	Not Quantified			Yes					Yes
57-55-6	1,2-Propylene glycol	110	mg/L	Yes	Yes	Yes				Yes
57-60-3	Pyruvate	Not Quantified			Yes					
57-88-5	Cholesterol	0.00026	mg/L		Yes					Yes
57-97-6	7,12-Dimethylbenz(a)anthracene	Not Quantified			Yes	Yes		Yes		Yes
58-08-2	Caffeine	0.0005	mg/L		Yes					Yes
581-40-8	2,3-Dimethylnaphthalene	Not Quantified			Yes					
581-42-0	2,6-Dimethylnaphthalene	Not Quantified			Yes					Yes
58175-57-8	1-Pentanol, 2-propyl-	Not Quantified								
582-16-1	2,7-Dimethylnaphthalene	Not Quantified								
584-02-1	3-Pentanol	Not Quantified			Yes					
58422-90-5	1,3-Dioxolane-2-heptanenitrile, ð-methyl-ð-oxo-2-phenyl-	Not Quantified								
5842-53-5	2,2,4-Trimethylpent-3-en-1-ol	Not Quantified								
58462-32-1	trans, trans-3-Ethylbicyclo[4.4.0]decane	Not Quantified								
588-16-9	3-Methoxyacetanilide	Not Quantified								
58-89-9	Lindane	Not Quantified			Yes	Yes	Yes	Yes	Yes	Yes
589-43-5	2,4-Dimethylhexane	Not Quantified			Yes					

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
589-53-7	4-Methylheptane	Not Quantified			Yes					
589-90-2	1,4-Dimethylcyclohexane	Not Quantified			Yes					
589-98-0	3-octanol	Not Quantified			Yes					
590-66-9	1,1-Dimethylcyclohexane	Not Quantified			Yes					
591-11-7	2(5H)-Furanone, 5-methyl-	Not Quantified								
591-21-9	1,3-Dimethylcyclohexane	Not Quantified			Yes					
591-48-0	3-Methylcyclohexene	Not Quantified								
591-78-6	2-Hexanone	1.07	mg/L		Yes	Yes				Yes
592-27-8	2-Methylheptane	Not Quantified			Yes					
59303-13-8	2-Methyl-5-propionylthiophene	Not Quantified								
593-45-3	Octadecane	0.28	mg/L		Yes					Yes
593-49-7	Heptacosane	0.00095	mg/L							
594-61-6	2-Hydroxyisobutyric acid	Not Quantified			Yes					
59473-04-0	Tox	3.88	mg/L							
594-91-2	Perfluoro-2-methylbutane	Not Quantified								
597-49-9	3-Pentanol, 3-ethyl-	Not Quantified								
598-89-0	Diiodoacetic acid	Not Quantified								
599-64-4	4-Cumylphenol	0.00118	mg/L		Yes					Yes
6006-33-3	Cyclohexane, tridecyl-	Not Quantified								
60186-80-3	5-Tridecyne	Not Quantified								
60212-33-1	4-Tetradecyne	Not Quantified								
60274-60-4	Pentane, 1-chloro-5-iodo-	Not Quantified								
6032-29-7	Pentan-2-ol	0.0087	mg/L		Yes					
6044-71-9	Dodecane, 6-methyl-	Not Quantified								
605-39-0	1,1'-Biphenyl, 2,2'-dimethyl-	Not Quantified								
60-57-1	Dieldrin	Not Quantified			Yes	Yes	Yes	Yes		Yes
6069-98-3	Cyclohexane, 1-methyl-4-(1-methylethyl)-, cis-	Not Quantified								
610-48-0	1-Methylantracene	0.00048	mg/L							
611-14-3	1-Ethyl-2-methylbenzene	0.0061	mg/L		Yes					Yes
61141-72-8	4,6-Dimethyldodecane	Not Quantified								
61141-80-8	Cyclohexane, 1,2-diethyl-3-methyl-	Not Quantified								
61142-19-6	(1,3-Dimethylbutyl)cyclohexane	Not Quantified								
61142-24-3	cyclohexane, 1,2,4,5-tetraethyl-, (1.alpha.,2.alpha.,4.alpha.	Not Quantified								
61142-32-3	Cyclopentene, 1,3-dimethyl-2-(1-methylethyl)-	Not Quantified								
61142-38-9	Cyclohexane, (3-methylpentyl)-	Not Quantified								
61142-52-7	1-Butyl-2-pentylcyclopentane	Not Quantified								
61142-66-3	cyclopentene, 5-hexyl-3,3-dimethyl-	Not Quantified								
61142-68-5	1-Hexyl-3-methylcyclopentane	Not Quantified								
61142-70-9	2,4-Diethyl-1-methylcyclohexane	Not Quantified								
61177-16-0	Bicyclo[2.2.1]heptane, 2-butyl-	Not Quantified								
6117-97-1	4-Methyldodecane	0.0101	mg/L							
61208-94-4	Cyclohexane, (1-methylbutyl)-	Not Quantified								
61233-71-4	1,6,9-tetradecatriene	Not Quantified								
613-33-2	4,4'-Dimethylbiphenyl	Not Quantified								
61413-70-5	Chloromethyl octanoate	Not Quantified								
615-22-5	2-(Methylthio)benzothiazole	0.00054	mg/L							Yes
615-43-0	o-Iodoaniline	Not Quantified								
6165-40-8	7-Methylpentadecane	Not Quantified			Yes					
6165-44-2	Cyclohexane, 1,1'-(1,4-butanediyl)bis-	Not Quantified								
61819-81-6	2,3',5'-Trimethyldiphenylmethane	0.00005	mg/L							
61886-62-2	3-Hexadecyne	Not Quantified								
61985-25-9	4-Acetylimidazole	Not Quantified								
619-99-8	3-Ethylhexane	Not Quantified			Yes					
620-14-4	3-Ethyltoluene	Not Quantified			Yes					
62016-19-7	octane, 6-ethyl-2-methyl-	Not Quantified			Yes					

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
62016-28-8	2,2,6-Trimethyloctane	Not Quantified			Yes					
62016-37-9	2,4,6-Trimethyloctane	Not Quantified			Yes					
62016-79-9	1-Chloroheptacosane	Not Quantified								
62108-21-8	Decane, 6-ethyl-2-methyl-	Not Quantified								
62108-25-2	Decane, 2,6,7-trimethyl-	Not Quantified								
62108-27-4	decane, 2,4,6-trimethyl-	Not Quantified								
621-42-1	3-Acetamidophenol	Not Quantified			Yes					
62183-55-5	3-Ethyl-2,7-dimethyloctane	Not Quantified								
62185-55-1	Nonane, 4-methyl-5-propyl-	Not Quantified								
62187-13-7	3-Octene, 2,2-dimethyl-, (E)-	Not Quantified								
62199-51-3	1-Pentyl-2-propylcyclopentane	Not Quantified								
62199-52-4	1,2-Dibutylcyclopentane	Not Quantified								
62238-11-3	2,3,5-Trimethyl-decane	Not Quantified								
62238-13-5	2,3,7-Trimethyldecane	Not Quantified								
62238-15-7	Decane, 2,3,4-trimethyl-	Not Quantified								
62238-29-3	cyclohexane, 1-ethyl-1,3-dimethyl-, trans-	Not Quantified								
62238-32-8	cyclohexane, 1-ethyl-1,4-dimethyl-, trans-	Not Quantified								
62238-33-9	cyclohexane, 1-ethyl-2-propyl-	Not Quantified			Yes					
623-55-2	3-Hexanol, 5-methyl-	Not Quantified								
62376-17-4	1,2-Dimethyl-3-pentyl-4-propylcyclohexane	Not Quantified								
624-29-3	Cyclohexane, 1,4-dimethyl-, cis-	Not Quantified								
6248-88-0	Bicyclo[2.2.1]heptane, 1,3,3-trimethyl-	Not Quantified								
625-31-0	4-Penten-2-ol	Not Quantified			Yes					
62583-58-8	1-Butyl-2-ethyloctahydro-1H-4,7-epoxyinden-5-ol	0.0009 mg/L								
626-03-9	2,4-Dihydroxypyridine	Not Quantified								
626-98-2	2-Pentenoic acid	Not Quantified								
629-50-5	Tridecane	0.0524 mg/L		Yes	Yes					
629-59-4	Tetradecane	0.948 mg/L		Yes	Yes					Yes
62960-77-4	4-Octene, 2,6-dimethyl-, [S-(Z)]-	Not Quantified								
629-62-9	Pentadecane	Not Quantified			Yes					
629-72-1	1-Bromopentadecane	Not Quantified								
629-73-2	1-Hexadecene	Not Quantified		Yes	Yes					
629-78-7	Heptadecane	Not Quantified			Yes					
629-80-1	Hexadecanal	0.165 mg/L								
629-89-0	Octadecyne	Not Quantified								
629-92-5	Nonadecane	Not Quantified			Yes					
629-94-7	Heneicosane	Not Quantified			Yes					
629-97-0	Docosane	0.224 mg/L			Yes					Yes
629-99-2	Pentacosane	0.00154 mg/L								
630-01-3	Hexacosane	0.0651 mg/L								Yes
630-02-4	Octacosane	0.0387 mg/L			Yes					Yes
630-03-5	Nonacosane	Not Quantified			Yes					
630-06-8	Hexatriacontane	Not Quantified								
630-07-9	Pentatriacontane	Not Quantified			Yes					
6305-52-8	2-n-Butyldecahydronaphthalene	Not Quantified								
63088-19-7	(4R*,5R*,9S*)-5,9-Dimethylspiro[3.5]nonan-1-one	Not Quantified								
63263-09-2	1,3-Dimethyladamantan-5-carboxylic acid, ethyl ester	Not Quantified								
63449-41-2	Benzyl-C8-18-alkyldimethylammonium chlorides	Not Quantified			Yes					
63521-76-6	Tridecanedial	0.00086 mg/L								
63798-30-1	2-Butynamide, N-methyl-	Not Quantified								
638-29-9	Valeryl chloride	Not Quantified								
63830-68-2	4-Nonene, 2,3,3-trimethyl-, (Z)-	Not Quantified								
638-36-8	2,6,10,14-Tetramethylhexadecane	0.0896 mg/L								
638-60-8	2-Tetradecene	Not Quantified								
638-66-4	Octadecanal	0.094 mg/L								

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
638-67-5	Tricosane	0.0017	mg/L							
638-68-6	Triacontane	0.0131	mg/L							Yes
64-17-5	Ethanol	0.5333	mg/L	Yes	Yes					Yes
6418-41-3	tridecane, 3-methyl-	Not Quantified			Yes					
6418-44-6	heptadecane, 3-methyl-	Not Quantified								
64-18-6	Formic acid	Not Quantified		Yes	Yes	Yes		Yes		
64-19-7	Acetic acid	1600	mg/L	Yes	Yes					Yes
64275-73-6	(Z)-5-Octen-1-ol	Not Quantified								
64341-49-7	1-Bromo-3-butene-2-ol	Not Quantified								
643-93-6	3-Methylbiphenyl	Not Quantified								
645-10-3	1,7-dimethyl-4-(1-methylethyl)cyclodecane	Not Quantified								
646-07-1	Pentanoic acid, 4-methyl-	3.456	mg/L		Yes					
646-31-1	Tetracosane	0.112	mg/L							Yes
65119-95-1	22-Tricosenoic acid	0.00043	mg/L							
65-85-0	Benzoic acid	1.03	mg/L	Yes	Yes	Yes				Yes
65996-50-1	1H-Pyrrolo[3,2-d]pyrimidine-2,4(3H,5H)-dione	Not Quantified								
66-25-1	Hexanal	Not Quantified			Yes					Yes
66542-51-6	Chloromethyl hexanoate	Not Quantified								
66552-62-3	Naphthalene, decahydro-1,5-dimethyl-	Not Quantified								
66660-37-5	Trans, trans-2-ethylbicyclo[4.4.0]decane	Not Quantified								
66660-38-6	cis, trans-2-Ethylbicyclo[4.4.0]decane	Not Quantified								
66660-42-2	cis, cis-3-ethylbicyclo[4.4.0]decane	Not Quantified								
66826-95-7	1-(Cyclohexylmethyl)-4-methylcyclohexane	Not Quantified								
6682-71-9	4,7-Dimethylindan	Not Quantified								
6708-17-4	Bicyclooctyl	Not Quantified								
6750-34-1	1-dodecanol, 3,7,11-trimethyl-	Not Quantified								
67-56-1	Methanol	428	mg/L	Yes	Yes	Yes				Yes
67-63-0	Isopropanol	83	mg/L	Yes	Yes	Yes				Yes
67-64-1	Acetone	21.7	mg/L	Yes	Yes	Yes				Yes
6765-39-5	1-Heptadecene	Not Quantified								
67-66-3	Chloroform	Not Quantified			Yes	Yes	Yes	Yes	Yes	Yes
6783-92-2	cyclohexane, 1,1,2,3-tetramethyl-	Not Quantified								
68-12-2	N,N-Dimethylformamide	519	mg/L	Yes	Yes	Yes				Yes
68139-30-0	1-Propanaminium, N-(3-aminopropyl)-2-hydroxy-N,N-dime	Not Quantified		Yes						
68140-01-2	N-[3-(Dimethylamino)propyl] coco amides	Not Quantified		Yes						
68213-23-0	Alcohols, C12-18, ethoxylated	0.3	mg/L							
68334-30-5	Fuels, diesel	1.3	mg/L		Yes					Yes
68593-94-2	2-Ethenylphenanthrene	0.00022	mg/L							
68603-15-6	Alcohols, C6-12	Not Quantified		Yes	Yes					
693-13-0	Diisopropylcarbodiimide	Not Quantified								
6937-34-4	3-iodophthalic acid	Not Quantified								
69462-10-8	2,2,4-Trimethylpentanenitrile	Not Quantified								
695-06-7	gamma-Caprolactone	Not Quantified			Yes					
69586-09-0	2,2-Dichloro-3,6-dimethyl-2H-1,2-oxasiline	Not Quantified								
696-29-7	Cyclohexane, (1-methylethyl)-	Not Quantified			Yes					
6971-40-0	17-pentatriacontene	0.001	mg/L							
6971-52-4	3-Methoxy-2-methylphenol	Not Quantified								
6975-98-0	2-Methyldecane	Not Quantified								
697-82-5	2,3,5-Trimethylphenol	Not Quantified			Yes					
6982-25-8	DL-2,3-Butanediol	Not Quantified								
69855-48-7	1-Methyl-4-(methylsulfonyl)bicyclo[2.2.2]octane	Not Quantified								
698-76-0	delta-Octanolactone	Not Quantified			Yes					
700000-97-1	2,3,3-Trimethyl-1-hexene	Not Quantified								
700-12-9	Benzene, pentamethyl-	0.2588	mg/L		Yes					Yes
702-79-4	1,3-Dimethyladamantane	9.8	mg/L							

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
7040-53-1	Dicyclohexyl methylphosphonate	Not Quantified								
7045-70-7	1,3-Diisopropyl cyclohexane	Not Quantified								
7045-71-8	2-Methylundecane	0.0703	mg/L							
705-86-2	6-Pentyltetrahydro-2H-pyran-2-one	Not Quantified			Yes					
706-14-9	gamma-Decanolactone	Not Quantified			Yes					
707-35-7	1,3,5-Trimethyladamantane	Not Quantified								
7098-21-7	Tritetracontane	Not Quantified								
7098-22-8	Tetratetracontane	Not Quantified								
71060-57-6	Alcohol ethoxylated*	Not Quantified		Yes	Yes					
71312-54-4	1,4-Dimethyl-2,3-diazabicyclo[2.2.1]hept-2-ene	Not Quantified								
71-36-3	1-Butanol	16.5	mg/L	Yes	Yes	Yes				Yes
71-43-2	Benzene	860	mg/L	Yes	Yes	Yes	Yes	Yes	Yes	Yes
7145-99-5	1,3-Benzodioxole, 5-methyl-	Not Quantified								
71-47-6	Formic acid, ion(1-)	Not Quantified								
71-50-1	Acetate	10037.65	mg/L							Yes
71-52-3	Bicarbonate	13900	mg/L		Yes					Yes
719-22-2	2,6-Bis-(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione	0.00028	mg/L							Yes
71940-29-9	3,4-Dimethyl-2-(3-methyl-butyl)-benzoic acid, methyl est	Not Quantified								
72-03-7	Propanoate	31.42096	mg/L							
7206-14-6	3-Dodecene, (E)-	Not Quantified								
7206-19-1	3-Octadecene, (E)-	Not Quantified								
7206-25-9	9-octadecene, (e)-	Not Quantified								
7216-42-4	Isonicotinaldehyde 1-oxide	Not Quantified								
72218-58-7	3-Methylheptyl acetate	Not Quantified								
72-55-9	p,p'-DDE	Not Quantified			Yes	Yes	Yes	Yes		Yes
73105-67-6	1-Iodo-2-methylundecane	Not Quantified								
7320-37-8	1,2-Epoxyhexadecane	Not Quantified			Yes					
7326-46-7	2-Furanol, tetrahydro-2-methyl-	Not Quantified								
73493-71-7	9-Methoxy-9H-fluorene	0.00018	mg/L							
7373-13-9	2-Octadecanone	0.215	mg/L							
74054-92-5	1,1,6,6-tetramethylspiro[4.4]nonane	Not Quantified								
7411-16-7	3-Ethyl-1,2,4(1H)-triazole	Not Quantified								
7421-93-4	Endrin aldehyde	Not Quantified			Yes		Yes			Yes
7429-90-5	Aluminum	686	mg/L	Yes	Yes	Yes				Yes
7429-91-6	Dysprosium	0.0004	mg/L		Yes					
74367-34-3	3-Hydroxy-2,4,4-trimethylpentyl 2-methylpropanoate	Not Quantified								
7439-89-6	Iron	2838	mg/L		Yes	Yes				Yes
7439-91-0	Lanthanum	0.00251	mg/L		Yes	Yes				Yes
7439-92-1	Lead	70.2	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
7439-93-2	Lithium	24600	mg/L		Yes	Yes				Yes
7439-94-3	Lutetium	0.00045	mg/L		Yes	Yes				
7439-95-4	Magnesium	13000	mg/L		Yes					Yes
7439-96-5	Manganese	931	mg/L		Yes	Yes				Yes
7439-97-6	Mercury	0.0138	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
7439-98-7	Molybdenum	11	mg/L		Yes	Yes				Yes
7439-99-8	Neptunium	1640	pCi/L							
7440-00-8	Neodymium	0.00051	mg/L		Yes					
7440-02-0	Nickel	4.78	mg/L	Yes	Yes	Yes		Yes		Yes
7440-10-0	Praseodymium	0.0004	mg/L		Yes					
7440-14-4	Radium	18045	pCi/L		Yes					Yes
7440-17-7	Rubidium	22.3	mg/L		Yes	Yes				Yes
7440-19-9	Samarium	0.0012	mg/L		Yes					
7440-20-2	Scandium	0.003	mg/L		Yes					Yes
7440-21-3	Silicon	160	mg/L	Yes	Yes					Yes
7440-22-4	Silver	2	mg/L		Yes	Yes	Yes	Yes		Yes

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
7440-23-5	Sodium	119000	mg/L	Yes	Yes					Yes
7440-24-6	Strontium	36000	mg/L		Yes	Yes				Yes
7440-27-9	Terbium	0.0004	mg/L		Yes					
7440-28-0	Thallium	10	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
7440-29-1	Thorium	35.9	mg/L		Yes					Yes
7440-30-4	Thulium	0.0004	mg/L		Yes					
7440-31-5	Tin	0.3341	mg/L		Yes	Yes				Yes
7440-32-6	Titanium	4.16	mg/L		Yes					Yes
7440-33-7	Tungsten	0.096	mg/L		Yes	Yes				Yes
7440-36-0	Antimony	12	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
7440-38-2	Arsenic	15	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
7440-39-3	Barium	160000	mg/L		Yes	Yes		Yes	Yes	Yes
7440-41-7	Beryllium	18.2	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
7440-42-8	Boron	176000	mg/L		Yes	Yes				Yes
7440-43-9	Cadmium	0.99	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
7440-44-0	Carbon	3750	mg/L	Yes	Yes					Yes
7440-45-1	Cerium	0.00041	mg/L		Yes					Yes
7440-46-2	Cesium	537	mg/L		Yes					Yes
7440-47-3	Chromium	83.9	mg/L		Yes		Yes	Yes	Yes	Yes
7440-48-4	Cobalt	8.2	mg/L		Yes	Yes				Yes
7440-50-8	Copper	24.2	mg/L		Yes	Yes	Yes		Yes	Yes
7440-52-0	Erbium	0.0004	mg/L		Yes					
7440-53-1	Europium	0.01317	mg/L		Yes					
7440-54-2	Gadolinium	0.00277	mg/L		Yes	Yes				
7440-56-4	Germanium	0.44	mg/L		Yes					Yes
7440-57-5	Gold	0.018	mg/L		Yes					Yes
7440-58-6	Hafnium	0.00545	mg/L		Yes					Yes
7440-60-0	Holmium	0.0004	mg/L		Yes					
7440-61-1	Uranium	497	pCi/L		Yes	Yes			Yes	Yes
7440-62-2	Vanadium	4.51	mg/L		Yes	Yes				Yes
7440-64-4	Ytterbium	0.00278	mg/L		Yes					
7440-65-5	Yttrium	0.011	mg/L		Yes					Yes
7440-66-6	Zinc	243	mg/L		Yes	Yes	Yes			Yes
7440-67-7	Zirconium	8.76	mg/L	Yes	Yes	Yes				Yes
7440-69-9	Bismuth	0.424	mg/L		Yes					Yes
7440-70-2	Calcium	180000	mg/L		Yes					Yes
74421-09-3	cyclopentane, 1,1,3-trimethyl-3-(2-methyl-2-propenyl)-	Not Quantified								
74630-16-3	Phosphonous dichloride, (1,7,7-trimethylbicyclo[2.2.1]hept	Not Quantified								
74646-31-4	14-Bromo-1-tetradecene	Not Quantified								
74646-37-0	1-Tridecyn-4-ol	Not Quantified								
74646-38-1	4,4-Dimethyltetracyclo[5.2.1.02.6.03,5]decane	0.00027	mg/L							
74663-66-4	Cyclohexane, 1,5-diethyl-2,3-dimethyl-	Not Quantified								
74663-71-1	cyclohexane, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-	Not Quantified								
74685-30-6	5-eicosene, (e)-	Not Quantified								
74685-33-9	3-eicosene, (e)-	Not Quantified								
74810-41-6	cyclohexane, (2-ethyl-1-methylbutylidene)-	Not Quantified								
74810-42-7	cyclohexane, (2-ethyl-1-methyl-1-butenyl)-	Not Quantified								
74-82-8	Methane	3420.48	mg/L		Yes					Yes
74-83-9	Methyl bromide	Not Quantified			Yes	Yes	Yes	Yes		Yes
74-84-0	Ethane	571.19	mg/L	Yes	Yes					
74-87-3	Chloromethane	0.0054	mg/L	Yes	Yes	Yes	Yes	Yes		Yes
74-98-6	Propane	86.92	mg/L	Yes	Yes					
75-07-0	Acetaldehyde	0.1	mg/L	Yes	Yes	Yes				Yes
75-09-2	Dichloromethane	0.51	mg/L	Yes	Yes	Yes	Yes	Yes	Yes	Yes
75-15-0	Carbon disulfide	Not Quantified			Yes	Yes		Yes		Yes

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CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
75163-97-2	octadecane, 2,6-dimethyl-	0.2917	mg/L							
7524-63-2	2,6-DIMETHYLTETRALINE	Not Quantified								
75-25-2	Bromoform	Not Quantified			Yes	Yes	Yes	Yes	Yes	Yes
75-27-4	Bromodichloromethane	Not Quantified			Yes	Yes	Yes		Yes	Yes
75-34-3	1,1-Dichloroethane	0.005	mg/L		Yes	Yes	Yes	Yes		Yes
754-43-8	2-Bromo-1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)propane	Not Quantified								
7553-56-2	Iodine	385	mg/L		Yes	Yes				Yes
75-65-0	tert-Butyl alcohol	0.071	mg/L		Yes					Yes
75-83-2	2,2-Dimethylbutane	0.00066	mg/L		Yes					
762-42-5	2-Butynedioic acid, dimethyl ester	Not Quantified								
7631-86-9	Silica	225	mg/L	Yes	Yes					Yes
76-44-8	Heptachlor	Not Quantified			Yes	Yes	Yes	Yes	Yes	Yes
764-96-5	(5Z)-5-Undecene	Not Quantified								
7664-41-7	Ammonia	1970	mg/L	Yes	Yes	Yes				Yes
766-76-7	Benzoate	0.3512364	mg/L							
767-58-8	Indan, 1-methyl-	Not Quantified								
7683-64-9	Squalene	0.00024	mg/L							Yes
7704-34-9	Sulfur	112	mg/L	Yes	Yes					Yes
7723-14-0	Phosphorus	4222	mg/L		Yes	Yes				Yes
7726-95-6	Bromine	259	mg/L		Yes					Yes
7727-37-9	Nitrogen	96026	mg/L	Yes	Yes					Yes
7773-83-3	1-Docosanethiol	Not Quantified								
7782-49-2	Selenium	17	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
77877-94-2	Chloromethyl pentanoate	Not Quantified								
779-02-2	9-Methylanthracene	Not Quantified			Yes					
77-90-7	Acetyl tributyl citrate	Not Quantified			Yes					
78-59-1	Isophorone	0.015	mg/L		Yes	Yes	Yes			Yes
78-67-1	Azobisisobutyronitrile	Not Quantified			Yes					
78-77-3	1-Bromo-2-methylpropane	Not Quantified			Yes					
78-93-3	Methyl ethyl ketone	0.51	mg/L		Yes	Yes		Yes		Yes
79-01-6	Trichloroethylene	2.68	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
79-03-8	Propanoyl chloride	Not Quantified			Yes					
79-06-1	Acrylamide	99.2	mg/L	Yes	Yes	Yes		Yes	Yes	Yes
790-82-9	4,4'-Diacetyldiphenylmethane	0.00037	mg/L							
79-09-4	Propionic acid	33	mg/L		Yes					Yes
79273-13-5	dispiro[4.2.4.2]tetradecane	Not Quantified								
79-31-2	2-Methylpropanoic acid	4	mg/L		Yes					
79-34-5	1,1,2,2-Tetrachloroethane	0.005	mg/L		Yes	Yes	Yes	Yes		Yes
8001-54-5	Benzalkonium chloride	1	mg/L	Yes	Yes					
80-05-7	Bisphenol A	0.01617	mg/L	Yes	Yes	Yes				Yes
80061-31-0	3,4-Dihydro-1,9(2H,10H)-acridinedione	0.00135	mg/L							
8008-20-6	Kerosine	0.2	mg/L	Yes	Yes	Yes				Yes
80625-32-7	1,e-8,z-10-pentadecatriene	Not Quantified								
80-62-6	Methyl methacrylate	0.03	mg/L		Yes	Yes		Yes		Yes
80655-44-3	Decahydro-4,4,8,9,10-pentamethylnaphthalene	Not Quantified								
821-55-6	2-Nonanone	Not Quantified			Yes					
82253-11-0	7-octylidenebicyclo[4.1.0]heptane	Not Quantified								
823-17-6	Cyclohexene, 3,5-dimethyl-	Not Quantified								
823-22-3	2H-Pyran-2-one, tetrahydro-6-methyl-	Not Quantified								
824-43-1	(1R,2S)-1,2-Diethylcyclohexane	Not Quantified								
825-44-5	Benzo(b)thiophene 1,1-dioxide	Not Quantified			Yes					
825-51-4	2-Naphthalenol, decahydro-	Not Quantified			Yes					
826-18-6	Benzene, 1-pentenyl-	Not Quantified								
82736-95-6	1,2,4-Triazine-3,5(2H,4H)-dione, 6-fluoro-	Not Quantified								
827-52-1	Cyclohexylbenzene	Not Quantified			Yes					

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
829-20-9	1-(2,4-Dimethoxyphenyl)ethan-1-one	Not Quantified								
829-26-5	2,3,6-Trimethylnaphthalene	Not Quantified			Yes					Yes
830-09-1	4-Methoxycinnamic acid	0.00016	mg/L							
83173-76-6	Benzenemethanol, 4-methyl-à-(1-methyl-2-propenyl)-, (R)	Not Quantified								
832-69-9	1-Methyl phenanthrene	0.000234	mg/L		Yes					Yes
83-32-9	Acenaphthene	0.28	mg/L		Yes	Yes	Yes			Yes
83-33-0	1H-Inden-1-one, 2,3-dihydro-	Not Quantified			Yes					
84-66-2	Diethyl phthalate	0.0149	mg/L		Yes	Yes	Yes	Yes		Yes
84-69-5	Diisobutyl phthalate	Not Quantified			Yes					Yes
84-74-2	Dibutyl phthalate	0.0151	mg/L		Yes	Yes	Yes	Yes		Yes
84-77-5	Didecyl phthalate	0.00723	mg/L		Yes					
85-01-8	Phenanthrene	1.2	mg/L		Yes		Yes			Yes
852228-22-9	1,54-Dibromotetrapentacontane	Not Quantified								
85-68-7	Benzyl butyl phthalate	0.0042	mg/L		Yes	Yes	Yes	Yes		Yes
85763-57-1	11-Methyldodecanol	Not Quantified								
86290-81-5	Gasoline	0.8	mg/L		Yes					Yes
86-30-6	N-Nitrosodiphenylamine	0.0017	mg/L		Yes	Yes	Yes			Yes
86-55-5	1-Naphthalenecarboxylic acid	0.96	mg/L		Yes					
866-23-9	Phosphonic acid, trichloromethyl-, diethyl ester	Not Quantified			Yes					
866760-27-2	(4Z)-2-Methyl-4-tetradecene	Not Quantified								
86-73-7	Fluorene	0.51	mg/L		Yes	Yes	Yes			Yes
871-83-0	2-Methylnonane	Not Quantified			Yes					
87-41-2	Phthalide	Not Quantified			Yes					
874-35-1	5-Methylindan	Not Quantified								
874-41-9	1,3-Dimethyl-4-ethylbenzene	Not Quantified			Yes					
87-61-6	1,2,3-Trichlorobenzene	0.0065	mg/L		Yes	Yes				Yes
87-65-0	2,6-Dichlorophenol	Not Quantified			Yes			Yes		Yes
877-44-1	1,2,4-Triethylbenzene	Not Quantified								Yes
879-12-9	1,2,3-Trimethylnaphthalene	0.004485087	mg/L							
88-18-6	2-tert-Butylphenol	Not Quantified			Yes					
89-16-7	Bis(8-methylnonyl) phthalate	Not Quantified								
89-18-9	Butyl 8-methylnonyl phthalate	Not Quantified								
89656-98-4	Cyclohexane, (2-methyl-1-propenyl)-	Not Quantified								
89-74-7	1-(2,4-Dimethylphenyl)ethanone	Not Quantified			Yes					
9000-30-0	Guar gum	Not Quantified		Yes	Yes					
90-12-0	1-Methylnaphthalene	0.003	mg/L		Yes	Yes				Yes
90548-09-7	Decahydro-1-methyl-2-methylenenaphthalene	Not Quantified								
90565-51-8	2-butyl-4-methyl-1,6-dihydro-6-pyrimidone	Not Quantified								
90832-26-1	4,5-Dihydro-à,à,4,4-tetramethyl-1H-pyrazole-1-propanol	Not Quantified								
90921-72-5	N-Allyl-p-hydroxybenzamide	Not Quantified								
91-17-8	Decalin	Not Quantified			Yes					
91-20-3	Naphthalene	88.4	mg/L	Yes	Yes	Yes	Yes	Yes		Yes
91-22-5	Quinoline	Not Quantified		Yes	Yes	Yes				Yes
91242-57-8	Cyclopentane, 1,2-dipropyl-	Not Quantified								
912629-93-7	(9E)-8-Methyl-9-tetradecen-1-yl acetate	Not Quantified								
91531-54-3	1,1,3a-trimethyl-1a,3a,5,6-tetrahydro-1h-cyclopropa[c]pent	Not Quantified								
91-57-6	2-Methylnaphthalene	110	mg/L		Yes	Yes				Yes
92013-16-6	1H-Indene, 2,3-dihydro-4-propyl-	Not Quantified								
92-51-3	Dicyclohexyl	Not Quantified			Yes					
92513-28-5	3-Methylquinoline-2-carboxylic acid	0.00665	mg/L							
92-52-4	Biphenyl	0.0242	mg/L	Yes	Yes	Yes				Yes
925-60-0	2-Propenoic acid, propyl ester	Not Quantified			Yes					
92-87-5	Benzidine	Not Quantified			Yes	Yes	Yes	Yes		Yes
930-89-2	(Z)-1-Ethyl-2-methylcyclopentane	Not Quantified								
93-09-4	2-Naphthalenecarboxylic acid	0.02582745	mg/L		Yes					

SI Table 4c: 1198 chemicals reported as being detected in produced water, summary data

CAS #	Name	Concentration data (Max Reported)	Units	FracFocus (2013-2017)	ToxvalDB	ToxVal (Restricted)	Priority Pollutant List	RCRA	NPDWS	Method exists?
931-36-2	2-Ethyl-4-methyl-1H-imidazole	Not Quantified								
932-40-1	trans-1,2-Diethyl cyclopentane	Not Quantified								
933-98-2	1-Ethyl-2,3-dimethylbenzene	Not Quantified			Yes					
934-34-9	Benzothiazolone	0.0039	mg/L							Yes
934-80-5	1,2-Dimethyl-4-ethylbenzene	Not Quantified			Yes					
93-53-8	Hydratropaldehyde	Not Quantified			Yes					
93-55-0	1-Phenylpropan-1-one	Not Quantified			Yes					
938-06-7	(4aS,8aR)-4a-Methyloctahydronaphthalen-2(1H)-one	Not Quantified								
93927-20-9	1-Ethyl-2-methylnaphthalene	0.00055	mg/L							
939-27-5	2-Ethyl-naphthalene	Not Quantified								Yes
941228-34-8	7-(Bromomethyl)pentadec-7-ene	0.00277	mg/L							
94492-10-1	2-Dimethylamino-4-methyl-pent-4-enenitrile	Not Quantified								
94-59-7	Safrole	Not Quantified			Yes	Yes		Yes		Yes
949-41-7	1a,9b-Dihydro-1H-cyclopropa[1]phenanthrene	Not Quantified								
95-16-9	Benzothiazole	0.01427	mg/L		Yes					Yes
95-47-6	o-Xylene	9430	mg/L		Yes				Yes	Yes
95-48-7	o-Cresol	7.76	mg/L		Yes	Yes				Yes
95-50-1	1,2-Dichlorobenzene	0.00068	mg/L		Yes	Yes	Yes	Yes	Yes	Yes
95-63-6	1,2,4-Trimethylbenzene	8730	mg/L	Yes	Yes	Yes				Yes
95-65-8	3,4-Dimethylphenol	Not Quantified			Yes	Yes				Yes
959028-24-1	4-Ethyl-2,3-dimethylhex-2-ene	Not Quantified								
95906-11-9	tris(2,4-di-tert-butylphenyl) phosphate	Not Quantified								
959103-74-3	Undecyl heptafluorobutanoate	Not Quantified								
95-93-2	1,2,4,5-Tetramethylbenzene	Not Quantified			Yes					
959-98-8	Endosulfan I	0.0005	mg/L		Yes					Yes
96-04-8	2,3-Heptanedione	Not Quantified								
96-76-4	2,4-Di-tert-butylphenol	0.004941527	mg/L		Yes					
97-72-3	Isobutyric anhydride	Not Quantified			Yes					
98060-54-9	Decane, trimethyl-	Not Quantified								
98-06-6	tert-Butylbenzene	86	mg/L		Yes	Yes				Yes
98-54-4	4-tert-Butylphenol	0.00019	mg/L		Yes					
98-82-8	Cumene	948	mg/L	Yes	Yes	Yes				Yes
98-86-2	Acetophenone	0.0011	mg/L	Yes	Yes	Yes		Yes		Yes
98-95-3	Nitrobenzene	0.006	mg/L		Yes	Yes	Yes	Yes		Yes
99-06-9	3-Hydroxybenzoic acid	0.03038684	mg/L		Yes					
99133-89-8	4-Imidazolacetic acid, butyl ester	Not Quantified								
99328-46-8	5-Methyl-1-hepten-4-ol	Not Quantified								
99-87-6	p-Cymene	334	mg/L		Yes					Yes
NOCAS_24858	m,p-Cresol mixture	Not Quantified								Yes
NOCAS_873040	Tricyclo[4.4.0.0(3,9)]decane	0.00026	mg/L							
NOCAS_873049	Tetrahydrophenanthrene	0.00042	mg/L							
NOCAS_873051	Ethyltetrahydronaphthalene	0.00046	mg/L							
NOCAS_891518	Nonylphenols	Not Quantified								

SI Table 5a: Summary of final 122 chemicals used for ToxPi prioritization based on availability of data: detected more than once; associated concentration data; having at least two types of toxicity data

Reflid	CAS #	Name	Concn (mg/L)	FracFocus (2013-2017)	Priority Pollutant List	RCRA	NPDWRs	Standard Method
5	100-41-4	Ethylbenzene	4410	Yes	Yes		Yes	Yes
9	100-42-5	Styrene	52				Yes	Yes
19	100-51-6	Benzyl alcohol	0.34					Yes
14	101-81-5	Diphenylmethane	0.00043					
5	103-65-1	Propylbenzene	1290					Yes
5	104-51-8	Butylbenzene	162					Yes
17	104-76-7	2-Ethyl-1-hexanol	0.041	Yes				Yes
15	105-60-2	Caprolactam	0.002392004					Yes
5	105-67-9	2,4-Dimethylphenol	5		Yes	Yes		Yes
10	106-42-3	p-Xylene	0.46				Yes	Yes
19	106-44-5	p-Cresol	0.3					Yes
17	106-46-7	1,4-Dichlorobenzene	0.00034		Yes	Yes	Yes	Yes
7	106-65-0	Dimethyl succinate	0.8914662	Yes				
17	107-21-1	Ethylene glycol	290	Yes				Yes
12	107-92-6	Butanoic acid	19					
16	108-10-1	4-Methyl-2-pentanone	1.44	Yes				Yes
17	108-38-3	m-Xylene	0.111	Yes			Yes	Yes
5	108-67-8	1,3,5-Trimethylbenzene	6250	Yes				Yes
5	108-88-3	Toluene	16800	Yes	Yes	Yes	Yes	Yes
5	108-95-2	Phenol	6.96	Yes		Yes		Yes
18	110-75-8	2-Chloroethyl vinyl ether	0.014		Yes	Yes		Yes
17	110-86-1	Pyridine	0.28			Yes		Yes
7	110-94-1	Glutaric acid	0.290653					
7	111-14-8	Heptanoic acid	0.3124488					
9	111-76-2	2-Butoxyethanol	77.5	Yes				Yes
17	1120-21-4	Undecane	0.0113	Yes				
17	112-30-1	1-Decanol	0.0054	Yes				
14	112-34-5	2-(2-Butoxyethoxy)ethanol	0.00045	Yes				
19	112-40-3	Dodecane	2.33	Yes				Yes
1	112-88-9	1-Octadecene	0.0463	Yes				
15	115-86-6	Triphenyl phosphate	0.00677137					Yes
19	117-81-7	Di(2-ethylhexyl) phthalate	0.042	Yes	Yes	Yes	Yes	Yes
17	117-84-0	Di-n-octyl phthalate	0.0093		Yes	Yes		Yes
7	118-90-1	2-Methylbenzoic acid	0.21784					
17	119-64-2	Tetralin	0.00895					
4	120-12-7	Anthracene	0.029		Yes			Yes
17	120-82-1	1,2,4-Trichlorobenzene	0.0015		Yes	Yes	Yes	Yes
7	121-91-5	1,3-Benzenedicarboxylic acid	0.3821036					
14	122-39-4	Diphenylamine	0.00373			Yes		Yes
7	123-25-1	Diethyl butanedioate	1.4109876					
12	123-91-1	1,4-Dioxane	0.06	Yes		Yes		Yes
7	124-07-2	Octanoic acid	0.08220198					
19	124-18-5	Decane	2.67	Yes				Yes
14	126-73-8	Tributyl phosphate	0.01896	Yes				Yes
17	127-18-4	Tetrachloroethylene	0.005		Yes	Yes	Yes	Yes
4	129-00-0	Pyrene	0.23		Yes			Yes
12	131-11-3	Dimethyl phthalate	0.015		Yes	Yes		Yes

SI Table 5a: Summary of final 122 chemicals used for ToxPi prioritization based on availability of data: detected more than once; associated concentration data; having at least two types of toxicity data

Reflid	CAS #	Name	Concn (mg/L)	FracFocus (2013-2017)	Priority Pollutant List	RCRA	NPDWRs	Standard Method
5	1319-77-3	Cresol	6.76			Yes		
19	132-65-0	Dibenzothiophene	0.0144					Yes
19	1330-20-7	Xylenes	11	Yes			Yes	Yes
5	135-98-8	sec-Butylbenzene	270					Yes
15	140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol	0.018338478					Yes
7	142-62-1	Hexanoic acid	0.766656					Yes
15	143-07-7	Dodecanoic acid	0.002517211					
4	191-24-2	Benzo(g,h,i)perylene	0.0015		Yes			Yes
4	193-39-5	Indeno(1,2,3-cd)pyrene	0.022		Yes	Yes		Yes
4	205-99-2	Benzo(b)fluoranthene	0.006		Yes	Yes		Yes
4	206-44-0	Fluoranthene	0.035		Yes	Yes		Yes
4	207-08-9	Benzo(k)fluoranthene	0.0049			Yes		Yes
4	208-96-8	Acenaphthylene	0.11		Yes			Yes
4	218-01-9	Chrysene	0.11		Yes	Yes		Yes
8	2381-21-7	1-Methylpyrene	0.0000477					Yes
15	28804-88-8	Dimethylnaphthalene	0.009506014					
17	319-86-8	delta-Hexachlorocyclohexane	0.000048		Yes			Yes
14	3386-33-2	Octadecyl chloride	0.00212					
17	496-11-7	Indan	0.0096					
4	50-32-8	Benzo(a)pyrene	0.035		Yes	Yes	Yes	Yes
18	503-74-2	Isovaleric acid	0.96					
4	53-70-3	Dibenz(a,h)anthracene	0.023		Yes	Yes		Yes
15	544-63-8	Tetradecanoic acid	0.005315497					
19	544-76-3	Hexadecane	0.601	Yes				Yes
4	56-55-3	Benz(a)anthracene	0.017		Yes	Yes		Yes
15	57-10-3	Hexadecanoic acid	0.003021193					
15	57-11-4	Octadecanoic acid	0.00373392					
17	57-55-6	1,2-Propylene glycol	110	Yes				Yes
17	611-14-3	1-Ethyl-2-methylbenzene	0.0061					Yes
17	629-50-5	Tridecane	0.0524	Yes				
19	629-59-4	Tetradecane	0.948	Yes				Yes
12	64-19-7	Acetic acid	1600	Yes				Yes
3	65-85-0	Benzoic acid	1.03	Yes				Yes
17	67-56-1	Methanol	428	Yes				Yes
17	67-63-0	Isopropanol	83	Yes				Yes
16	67-64-1	Acetone	21.7	Yes				Yes
5	71-43-2	Benzene	860	Yes	Yes	Yes	Yes	Yes
5	75-09-2	Dichloromethane	0.51	Yes	Yes	Yes	Yes	Yes
17	75-34-3	1,1-Dichloroethane	0.005		Yes	Yes		Yes
6	7553-56-2	Iodine	385					Yes
2	7631-86-9	Silica	225	Yes				Yes
19	78-93-3	Methyl ethyl ketone	0.51			Yes		Yes
12	79-09-4	Propionic acid	33					Yes
11	79-31-2	2-Methylpropanoic acid	4					
18	79-34-5	1,1,2,2-Tetrachloroethane	0.005		Yes	Yes		Yes
14	80-05-7	Bisphenol A	0.01617	Yes				Yes
18	80-62-6	Methyl methacrylate	0.03			Yes		Yes

SI Table 5a: Summary of final 122 chemicals used for ToxPi prioritization based on availability of data: detected more than once; associated concentration data; having at least two types of toxicity data

RefId	CAS #	Name	Concn (mg/L)	FracFocus (2013-2017)	Priority Pollutant List	RCRA	NPDWRs	Standard Method
8	832-69-9	1-Methyl phenanthrene	0.000234					Yes
4	83-32-9	Acenaphthene	0.28		Yes			Yes
14	84-66-2	Diethyl phthalate	0.0149		Yes	Yes		Yes
19	84-74-2	Dibutyl phthalate	0.0151		Yes	Yes		Yes
14	84-77-5	Didecyl phthalate	0.00723					
4	85-01-8	Phenanthrene	1.2		Yes			Yes
12	85-68-7	Benzyl butyl phthalate	0.0042		Yes	Yes		Yes
17	86-30-6	N-Nitrosodiphenylamine	0.0017		Yes			Yes
4	86-73-7	Fluorene	0.51		Yes			Yes
17	87-61-6	1,2,3-Trichlorobenzene	0.0065					Yes
18	90-12-0	1-Methylnaphthalene	0.003					Yes
13	91-20-3	Naphthalene	88.4	Yes	Yes	Yes		Yes
5	91-57-6	2-Methylnaphthalene	110					Yes
19	92-52-4	Biphenyl	0.0242	Yes				Yes
14	95-16-9	Benzothiazole	0.01427					Yes
5	95-47-6	o-Xylene	9430				Yes	Yes
5	95-48-7	o-Cresol	7.76					Yes
17	95-50-1	1,2-Dichlorobenzene	0.00068		Yes	Yes	Yes	Yes
5	95-63-6	1,2,4-Trimethylbenzene	8730	Yes				Yes
17	959-98-8	Endosulfan I	0.0005					Yes
15	96-76-4	2,4-Di-tert-butylphenol	0.004941527					
5	98-06-6	tert-Butylbenzene	86					Yes
14	98-54-4	4-tert-Butylphenol	0.00019					
5	98-82-8	Cumene	948	Yes				Yes
17	98-86-2	Acetophenone	0.0011	Yes		Yes		Yes
18	98-95-3	Nitrobenzene	0.006		Yes	Yes		Yes
7	99-06-9	3-Hydroxybenzoic acid	0.03038684					
5	99-87-6	p-Cymene	334					Yes

SI Table 5b: Reference IDs

RefId	Citation
1	Bell, E.A., Poynor, T.E., Newhart, K.B., Regnery, J., Coday, B.D., Cath, T.Y., 2017. Produced water treatment using forward osmosis membranes: Evaluation of extended-time performance and fouling. <i>Journal of Membrane Science</i> 525, 77–88. https://doi.org/10.1016/j.memsci.2016.10.032
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SI Table 5b: Reference IDs

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