

Non-target screening and prioritization of organic contaminants in seawater desalination brine using comprehensive two-dimensional gas chromatography-mass spectrometry

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ABSTRACT

With the expansion of seawater desalination, the impact of desalination brine on the marine environment attracts increasingly concerning globally. Salinity is generally accepted as the major environmental factor in desalination concentrate. However, more and more studies have shown people cannot ignore the influence of organic contaminants in brine. This study developed a non-targeted screening method based on comprehensive two-dimensional gas chromatography-quadrupole mass spectrometry combined with EPI Suite™ Toolbox 4.11 for identifying and prioritizing organic contaminants in the desalination brine. A total of 55 compounds were tentatively identified, including two polycyclic aromatic hydrocarbons, three engineering plastic ingredients, nine pesticides, eight plasticizers, two disinfection by-products, four phosphate ester flame retardants, two chlorophenols, and 25 other industry intermediates. We prioritize these chemicals by persistence (P), bioaccumulation (B), and toxicity (T) to determine whether they are harmful and need to be further analyzed. In addition, we found that four chemicals (caprolactam, N-phenyl-formamide, 2,4,6-tribromophenol, and tribromomethane) were possibly introduced from the desalination process. The method and results given in this study provide us with a new idea to identify the environmental impact factors of brine.

Keywords: Comprehensive two-dimensional gas chromatography-quadrupole mass spectrometry (GC × GC-qMS); Seawater desalination brine; Non-target screening; Environmental impact

1. Introduction

The water shortage is a global problem. With the development of the economy and population growth, the water demand-supply gap is expanding fast. It is estimated

that about 4 billion people are suffering from water shortages, and by 2050 this number will increase by 685 million [1]. Seawater desalination is increasingly important in narrowing the water demand-supply gap. The global desalination capacity has risen to 8.4×10^7 m³/d by 2022 [2].

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Desalination brine is the by-product of the seawater desalination process. With the rapid expansion of seawater desalination capacity, the volume of desalination brine is rising fast and gaining increasing concern [3]. Desalination brine can reduce the abundance assemblage structure of marine species, such as meiofauna [4–6], fishes [7,8], planktonic organisms [9], coral [10,11], seagrass [12], etc. Therefore, many countries, such as the United States, European Union, Australia, etc., have established relevant regulatory measures [13–15].

Salinity is generally considered the major environmental factor in desalination concentrate [16–20]. However, some studies showed that compounds in desalination brine could also significantly harm marine ecosystems [9,21]. The first reason is that the desalination process will nearly double the concentration of contaminants in raw seawater and discharge them into the ocean again. All manufactured chemicals, such as plastics, pesticides, fertilizers, pharmaceutical chemicals, etc. has been found in the ocean [22,23]. Pollution is more severe along coastlines where the desalination plants are based. Meanwhile, water treatment agents and their impurities or by-products added in the desalination process will also be introduced into the brine. Some water treatment agents contain nutrient elements such as nitrogen and phosphorus, increasing the abundance of organisms in the receiving water after discharge [24]. Some water treatment agents, for example, scale inhibitors, have a direct impact on the growth and development of coral [25,26], as well as on the diversity and community structure of marine microorganisms [27,28]. These compounds in desalination brine are always unknown (e.g., contaminants in seawater) or not given [29] (e.g., ingredients of commercial water treatment agents). Therefore, it is necessary to establish a non-target screening method for pollutants in desalination concentrate.

Comprehensive two-dimensional gas chromatography (GC × GC) is an effective technology in non-target analysis because of the high peak capacity and selectivity relative to conventional one-dimensional separations [30]. It has been used in the contaminants screening and identification of wastewater [31], biological samples [32], drinking water [33], etc. GC × GC-MS provides three-dimensional information for compounds (mass spectrogram, 1D retention time, and 2D retention time), which can improve the identification accuracy. Li et al. [33] investigated the accuracy of compound identification by two-dimensional gas chromatography-quadrupole mass spectrometry (GC × GC-qMS). Results showed that about 90% (41 of the 47) of the compounds automatically identified using the library were correct.

This study developed a non-target analysis method based on GC × GC-qMS combined with EPI Suite™ Toolbox 4.11 to screen and prioritize organic contaminants in the seawater desalination brine. GC × GC-MS can detect thousands of peaks. We used these peaks as fingerprints to compare raw seawater and brine and find new-introduced chemicals. This can give an overall information on the pollution increase because of desalination. To further explore the possible environmental risk, the peaks from brine were tentatively identified based on three-dimensional information (mass spectrum, 1D retention time, and 2D retention

time). Then, the identification results are prioritized by PBT (persistence, bioaccumulation, and toxicity).

2. Materials and method

2.1. Water samples

Tianjin Dagang desalination plant in Tianjin, China, started operation in 2009. It adopted reverse osmosis technology with a capacity of 100,000 m³/d. Its raw seawater is the cooling water from a power station. The water sample was collected from the inlet and outlet of the desalination plant in August 2022 and then filtered by 0.45 μm glass filter membrane and refrigerated at 4°C. The experiment would be conducted within a week.

2.2. Extraction procedure

The extraction process adopted from Bu et al. [34]. Each water sample (2 L) was concentrated by passing it through a 100 mg C18 solid phase extraction cartridge (Supelco, Bellefonte, USA) coupled to a 500 mg HLB cartridge (Waters, Milford, USA). The cartridges were conditioned before use with methyl tert-butyl ether, methanol, and water (10 mL each). The sample was passed through the tandem cartridges at a flow rate of 3–5 mL/min. The analytes were eluted using 10 mL of methyl tert-butyl ether, and then the eluents were dried over anhydrous sodium sulfate. Finally, the organic eluents were collected, concentrated to 0.1 mL under high-purity nitrogen, and reconstituted with *n*-hexane to 0.5 mL for GC × GC-qMS analysis. Each sample was conducted in duplicate. The control sample of raw water (before the reaction) was also analyzed under the same experimental procedures.

2.3. Analytical methods

Non-target analysis was performed using GC × GC-qMS. The gas chromatography was an Agilent 7890A (Agilent, USA). Agilent 5975C MSD mass spectrometer (Agilent, USA) was used as the detector. The comprehensive two-dimensional separation was achieved using Zoex ZX2 modulator (Zoex, USA). The first one-dimensional column was DB-5ms (30 m × 0.25 mm × 0.25 μm, Agilent, USA), and the two-dimensional column was BPX50 (2 m × 0.1 mm × 0.1 μm, SGE, Australia). Data processing was finished by GC Image Release 2.1 (Zoex, USA).

The injector temperature was set at 300°C with an injection volume of 1 μL. The gas chromatography (GC) temperature program began at 40°C, then increased to 300°C at the rate of 2.5°C/min and held for 10 min, then increased to 320°C at the rate of 2.5°C/min. The modulation period was 8 s, the initial temperature of the hot nozzle was 80°C. The hot pulse time was 400 ms, and the nitrogen cooling rate was 5 L/min. An electron impact (EI) ionization energy of 70 eV was selected. The scanning rate of mass spectrometry was 12,500 amu/s. Mass spectra were collected from *m/z* 50 to 500 with a data acquisition rate of 19.8 Hz. *N*-alkane mixed standard sample (C7-C28) was injected after sample injection to calculate the retention index of the compounds in the samples.

2.4. Data processing and compounds identification

The raw data obtained from GC × GC-qMS are first processed by GC Image software, including baseline removal, peak detection, and NIST library search. Then, the alkane matrix and column loss are removed from the chromatogram. Alkane compounds generally gather as an obvious band in the 2D retention time between 0–2 s, making identifying it easy. Column loss is usually silane compounds, of which the mass spectrogram characteristics can be easily distinguished. After the above processing, features in TIC were tentatively identified by NIST-05 library match. Reliable identification results can be obtained when setting the similarity cut-off as forward matching (M) > 700 and reverse matching (RM) > 800 [35,36]. However, the match similarity of contaminants in environmental matrices usually decreases due to many compounds with varying chemical properties typically present in the sample simultaneously. Therefore, we set the similarity cut-off as M > 600 and RM > 700 in this study. We use the retention index to identify library match results to increase the identification accuracy. Compounds would be removed if the difference in retention index between calculate and reference was more than 2%. If the reference retention index cannot be found for a result, we will match it again in NIST-05 library. The similarity criteria would be increased to M > 700 and RM > 800. All results that pass the above filters will be rechecked manually and confirmed by reference standards.

2.5. Chromatogram compare and new-introduced contaminants identification

The strong separation and peak capacity of GC × GC make it possible to compare the organic contaminant composition between in-take water and brine. Sources of newly introduced pollutants in desalinate concentrate include the

increase of the concentration of contaminants above the detection level and chemicals from the treatment process. Our previous experiments showed that 1D and 2D retention times had good repeatability [37]. In this study, each chromatographic peak was regarded as a coordinate point, and the horizontal and vertical coordinates were 1D and 2D retention time, respectively. Then, we put every coordinate point in the brine into the chromatogram of raw seawater and calculated its spatial distance with every peak in the chromatogram. In theory, the spatial distance of the same compound in both chromatograms would be zero. If a peak has a considerable spatial distance compared with all peaks in the seawater, this peak is from a new-introduced chemical in high possibility. Then this chemical will be further identified by chromatogram, retention index, and reference material. The schematic diagram can be found in supplementary data. The following formula calculates the space distance:

$$S = \sqrt{(RT'_1 - RT_1)^2 + (RT'_2 - RT_2)^2}$$

where S is the spatial distance of peak between brine and raw seawater. RT'_1 is the one-dimensional retention time of the chromatographic peak in brine, RT_1 is the 1D retention time of the chromatographic peak in raw seawater, RT'_2 is the 2D retention time of the chromatographic peak in raw seawater, and RT_2 is the 2D retention time of the chromatographic peak in raw seawater.

3. Results and discussion

3.1. Regulated contaminants

As shown in Table 1, Most regulated contaminants of desalination brine are higher than that of raw seawater.

Table 1
Regulated contaminants concentration in brine and seawater

	Seawater	Brine	Seawater criteria ^a	Discharge criteria ^b
pH	8.28	8.22	7.8–8.5 (I)	6.5–8.5
DO, mg/L	7.8	8.08	/	/
ORP, mv	180.1	140.3	/	/
TIN	0.39	1.31	0.5 (VI)	/
NH ₄ ⁺ , mg/L	0.11	0.93	/	/
NO ₂ ⁻ , mg/L	0.03	0.02	/	/
NO ₃ ⁻ , mg/L	0.25	0.36	/	/
TP, mg/L	0.02	0.49	0.045 ^c (VI)	0.5
TN, mg/L	1.04	1.21	/	/
Zn, μg/L	0.078	0.12	20 (I)	/
Cd, μg/L	0.065	0.068	1 (I)	/
Cr, μg/L	1.46	5.92	50 (I)	50
Ni, μg/L	0.55	0.61	5 (I)	/

^aSeawater Quality Standard of China (GB-3097-1997) [38] China classifies seawater quality into four categories (I, II, III, IV, from best to worst) based on use, each with different water quality requirements;

^bRequirements for discharge of seawater desalination brine (HY/T0289-2020) [39];

^cThis parameter is “reactive phosphate” in the standard instead of TP in this study;

^dChina divided seawater into four levels based on quality. VI seawater is the lowest requirement for seawater.

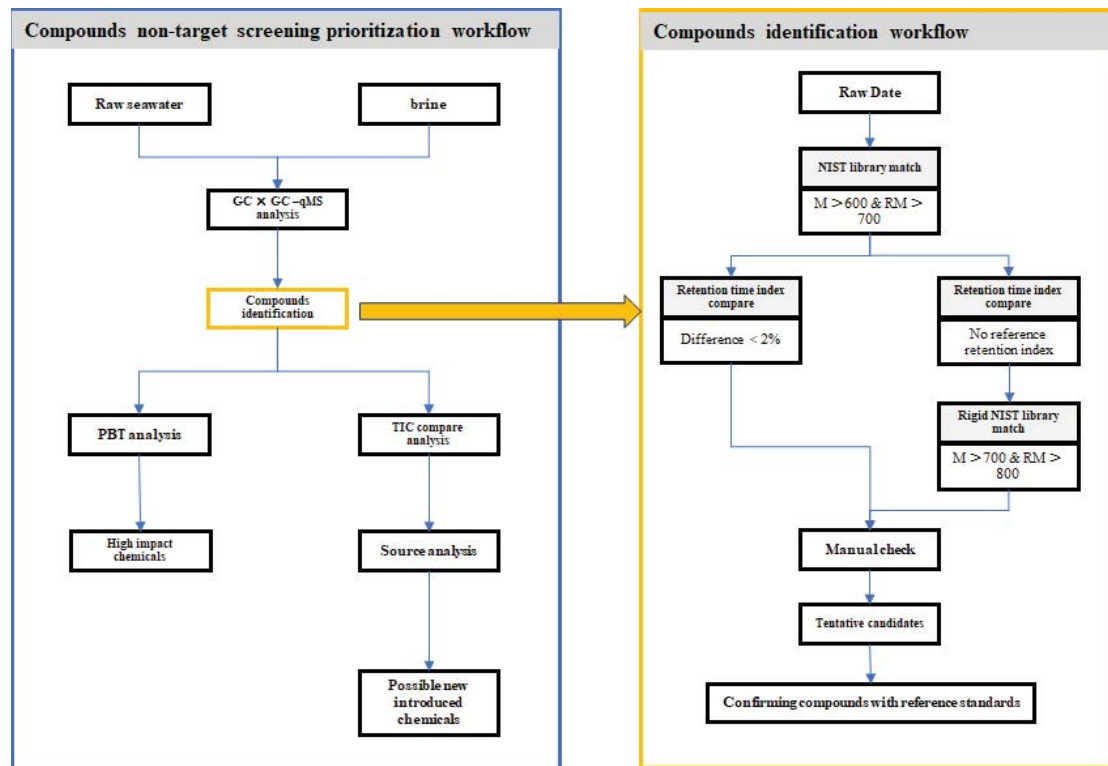


Fig. 1. Non-target analysis procedure of GC \times GC-qMS.

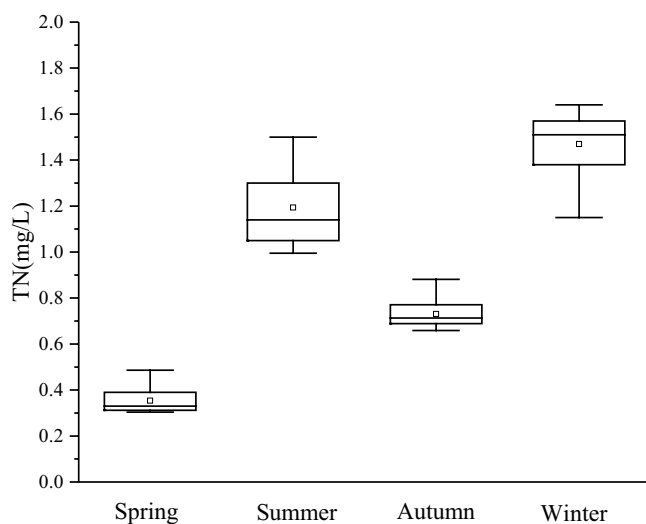


Fig. 2. Monitoring results of total nitrogen around the desalination plant in 2015.

The total inorganic nitrogen (TIN) concentration in brine was 1.31 mg/L, about 2.6 times the Chinese seawater quality criteria. Total phosphorus (TP) is slightly higher than the criteria. The main reason is that nitrogen in the seawater is very high. In 2015, we monitored the total nitrogen (TN) of seawater around the plant for 1 y. The results showed that the average TN concentration in spring, summer, autumn, and winter was 0.35, 1.19, 0.73, and 1.47 mg/L, respectively.

The main reason is that surface runoff is the primary TN source in Bohai Bay. More TN is introduced by surface runoff because of more rainfall in summer. In winter, there is more TN accumulated in the dry season. Zn, Cd, Gr, Ni concentration levels are below the requirement for I categories of seawater. Zn, Cd, Gr, Ni are the main corrosion products in thermal desalination plants and are possibly introduced by the desalination process. In this study, the concentration increase of these contaminants was about two times. The increase ratio was close to the recovery rate of the desalination process, so they were mainly from the enrichment of the desalination process instead of corrosion.

3.2. Compounds identification and prioritization

As shown in Fig. 3, 1,560 chromatographic peaks were detected in desalination concentrate and 1,535 in raw seawater. A total of 55 compounds were tentatively identified, including two polycyclic aromatic hydrocarbons, three engineering plastic ingredients, nine pesticides, eight plasticizers, two disinfection by-products, four phosphate ester flame retardants, two chlorophenols, and 25 other industry intermediates, which can be found in Table 2. The desalination process concentrated the contaminants in the seawater, so their concentration in brine is significantly higher than in raw seawater. For example, myclobutanil is only detected in brine. The reason is the desalination process increases its concentration above the detection limit. Tribromomethane and tribromophenol are only found in brine. They are mainly from the pre-treatment, where raw seawater is disinfected to control biofouling.

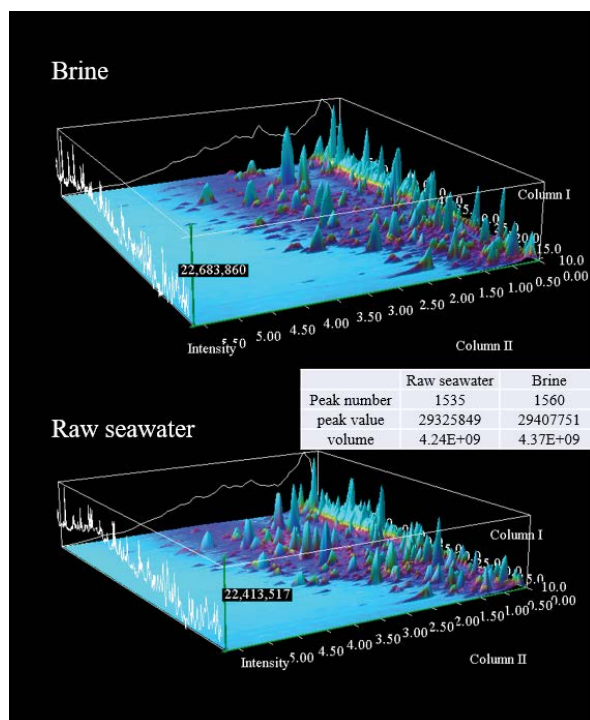


Fig. 3. GC × GC-qMS chromatogram of raw seawater and brine.

All the compounds identified in this study have not been included in the China seawater quality standard [38] or requirements for the discharge of seawater desalination brine in China [39]. Therefore, we prioritize these chemicals by persistence (P), bioaccumulation (B), and toxicity (T) to determine whether they are harmful and need to be further analyzed, which is an effective strategy to evaluate the potential environmental impact of commercial chemicals [40]. Aquatic toxicity (ChV), half-lives in water, and BCFs were estimated for each identified compound using the ECOSAR, BIOWIN3, and BAFBCF modules in the EPI Suite™ Toolbox 4.11 (<https://www.epa.gov/tsca-screening-tools/epi-suite-estimation-program-interface>).

The three pollutants with the longest half-life are bromomethane, 2,4,6-tribromophenol, and dimethyl phthalate. The three highest BCF were 2,4,6-tribromophenol, fluorenone, and naphthalene. The toxicity assessment adopted mysid of seawater as the endpoint. If there was no relevant data, fish in seawater was selected as the endpoint. When the above data was absent, fish in freshwater was chosen as the endpoint. The three most toxic compounds were bis(2-ethylhexyl) phthalate (DEHP), cyclohexyl isothiocyanate, and prometryn. It was considered that the compound is persistent and bioaccumulative if it has a half-life ($T^{1/2}$) > 180 [41] and BCF > 5,000 [41] (or 2,000 [42]). The pollutants identified in this study did not show obvious POPs characteristics.

Table 2
Compounds identified in desalination brine and their persistence, bioaccumulation, and toxicity prediction results

No.	Class	Identified chemical	CAS	Half-life (d)	ChV (ppm)	BCF	Endpoint
1	Polycyclic aromatic hydrocarbon	9,10-Anthracenedione	84-65-1	7.138	0.234	99.4	Mysid (seawater)
2		Naphthalene	91-20-3	0.495	0.245	177.2	Mysid (seawater)
3	Engineering plastics ingredient	Caprolactam	105-60-2	0.582	0.236	1.097	Fish (freshwater)
4		Diphenyl sulfone	127-63-9	12.829	2.297	18.77	Mysid (seawater)
5		Sulfone, methyl phenyl	3112-85-4	7.238	814.492	1.127	Mysid (seawater)
6	Pesticide	Prometryn	7287-19-6	0.281	0.057	53.51	Mysid (seawater)
7		Diethyltoluamide	134-62-3	0.423	0.075	13.3	Fish (freshwater)
8		Ametryn	834-12-8	0.375	0.176	29.85	Mysid (seawater)
9		Myclobutanil	88671-89-0	1.52	0.526	89.87	Mysid (seawater)
10		Simetryn	1014-70-6	0.563	0.541	23.7	Mysid (seawater)
11		Atrazine	1912-24-9	0.391	0.687	18.89	Mysid (seawater)
12		Acetochlor	34256-82-1	0.216	1.17	47.99	Fish (seawater)
13		Metolachlor	51218-45-2	0.191	1.437	39.22	Fish (seawater)
14		Desethylatrazine	6190-65-4	0.578	11.478	2.649	Mysid (seawater)
15		Bis(2-ethylhexyl) phthalate (DEHP)	117-81-7	0.487	6.78E-08	121.9	Mysid (seawater)
16		N-butylbenzenesulfonamide	3622-84-2	0.773	0.079	16.47	Fish (freshwater)
17		Dibutyl phthalate	84-74-2	1.153	0.141	159.4	Mysid (seawater)
18		Diisobutyl phthalate	84-69-5	1.155	0.252	25.67	Mysid (seawater)
19		Phthalic anhydride	85-44-9	14.276	7.986	4.879	Mysid (seawater)
20		Dimethyl phthalate	131-11-3	18.642	8.553	1.953	Fish (seawater)
21		Butyl citrate	77-94-1	0.667	34.314	6.376	Mysid (seawater)
22		Diethyl phthalate	84-66-2	3.086	257.6	5.889	Mysid (seawater)
23	Disinfection by-product	Phenol, 2,4,6-tribromo-	118-79-6	22.525	0.175	186.8	Fish (freshwater)
24		Tribromomethane	75-25-2	251.157	31.811	19.49	Mysid (seawater)

Table 2 (Continued)

Table 2

No.	Class	Identified chemical	CAS	Half-life (d)	ChV (ppm)	BCF	Endpoint
25	Phosphate ester	2-Propanol, 1-chloro-, phosphate (3:1)	13674-84-5	0.239	3.221	12.81	Mysid (seawater)
26	flame retardant	Tris(2-chloroethyl) phosphate	115-96-8	0.486	13.041	3.465	Fish (seawater)
27		Tributyl acetyl citrate	77-90-7	0.74	0.732	12.58	Mysid (seawater)
28		Triethyl phosphate	78-40-0	0.185	21.177	1.4	Fish (seawater)
29	Chlorophenols	Chloroxylenol	88-04-0	0.16	0.369	54.54	Fish (freshwater)
30		2,4-Dichlorophenol	120-83-2	3.588	0.79	33.95	Fish (freshwater)
31	Others	Isothiocyanato cyclohexane	1122-82-3	1.07	0.023	135.4	Mysid (seawater)
32		Benzene, 1,1'-[1,2-ethanediy]bis(oxy)]bis-	104-66-5	0.188	0.059	134.2	Mysid (seawater)
33		9H-Fluoren-9-one	486-25-9	1.732	0.108	181.5	Mysid (seawater)
34		Formamide, N-phenyl-	103-70-8	0.251	0.155	1.442	Fish (freshwater)
35		Benzothiazole	105-60-2	0.582	0.236	1.097	Fish (freshwater)
36		Benzophenone	119-61-9	3.009	0.372	23.93	Mysid (seawater)
37		1-Methyl-2-pyrrolidinone	872-50-4	0.486	0.446	0.9064	Fish (freshwater)
38		(1-Hydroxycyclohexyl)phenylmethanone	947-19-3	0.708	0.946	15.98	Fish (freshwater)
39		1,3,5-Trimethyl-1,3,5-triazinane-2,4,6-trione	827-16-7	2.289	1.053	3.811	Mysid (seawater)
40		Benzaldehyde	100-52-7	0.599	1.41	3.566	Fish (seawater)
41		4-Methoxybenzaldehyde	123-11-5	0.431	1.663	6.613	Fish (seawater)
42		Benzoic acid, 4-ethoxy-, ethyl ester	23676-09-7	0.723	1.899	87.53	Fish (seawater)
43		Benzyl nitrile	140-29-4	5.172	3.155	3.334	Fish (freshwater)
44		Phenol	108-95-2	0.32	3.605	2.419	Fish (freshwater)
45		1H-Pyrrole-2,5-dione, 3-ethenyl-4-methyl-	20189-42-8	0.529	3.677	3.32	Fish (freshwater)
46		1,6-Dioxacyclododecane-7,12-dione	777-95-7	1.065	4.261	3.142	Fish (freshwater)
47		2,3-Dihydro-1H-inden-1-one	83-33-0	1.465	6.316	13.11	Mysid (seawater)
48		Benzyl benzoate	120-51-4	1.535	7.39	19.15	Mysid (seawater)
49		4,5,6,7-Tetrahydro-benzofurazan	273-09-6	1.188	10.866	5.062	Mysid (seawater)
50		2,6,6-Trimethyl-2-cyclohexene-1,4-dione	1125-21-9	0.144	13.518	6.214	Mysid (seawater)
51		Benzyl alcohol	100-51-6	1.296	15.538	1.549	Fish (freshwater)
52		Triphenylphosphine oxide	791-28-6	1.829	18.54	46.5	Fish (freshwater)
53		1(3H)-Isobenzofuranone	87-41-2	0.24	18.913	1.222	Fish (seawater)
54		Acetophenone	98-86-2	5.691	21.501	3.928	Mysid (seawater)
55		Hedione	24851-98-7	0.501	71.724	17.77	Mysid (seawater)

Aquatic toxicity (ChV), half-lives in water, and BCFs were estimated for each identified compound using the ECOSAR, BIOWIN3, and BAFBCF modules in the EPI Suite™ Toolbox 4.11 (<https://www.epa.gov/tsc-screening-tools/epi-suite-estimation-program-interface>)

3.3. Chromatogram compare and new-introduced contaminants identification

As shown in Fig. 3, 1,560 chromatographic peaks were detected in desalination concentrate and 1,535 in raw seawater. Compared with raw seawater, the total peak value and peak volume of desalination concentrate increased slightly by about 0.3% and 3%, respectively. Among them, 496 chromatographic peaks coincided completely, accounting for about 32%. This is a very rough and tentative screening. However, the method will provide a direction for further screening new-introduced chemicals.

The recovery rate of the seawater desalination plant is about 40%, which can double the concentration of seawater contaminants in theory. Therefore, compounds whose concentration changes between seawater and brine above 100% will likely be pollutants introduced by the treatment process. Consequently, we set the peak volume or value

change's cut-off as 100%. Fig. 5 shows five contaminants passed the filter: caprolactam, myclobutanil, 2,4,6-tribromophenol, tribromomethane, and N-phenyl-formamide.

2,4,6-Tribromophenol and tribromomethane were only detected in desalination concentrate, which may come from the disinfection process of pre-treatment. Due to high bromide concentrations in seawater, highly brominated DBPs will form, which is more cytotoxic and genotoxic [43]. This result is similar to research in 2017. Yang et al. [44] monitored a seawater desalination plant in the same region. The results shown that the concentrations of trihalomethanes (THMs), haloacetic acids (HAAs), and haloacetonitriles (HANs) increased by 35.1, 23.7 and 4.9 µg/L, respectively, and brominated DBPs was the main species of THMs. Myclobutanil was also only detected in brine. It is a commercial pesticide used as a fungicide. Therefore, there is little possibility to be introduced from the desalination process. It was more likely from the raw seawater, and the

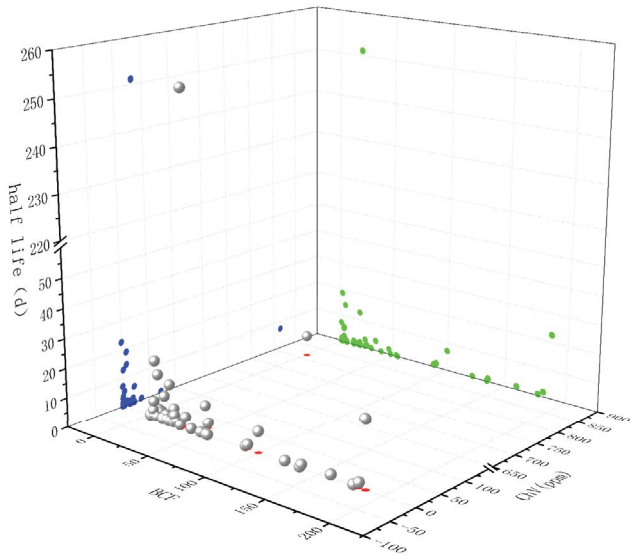


Fig. 4. Persistence, bioaccumulation, and toxicity analysis of identified chemicals.

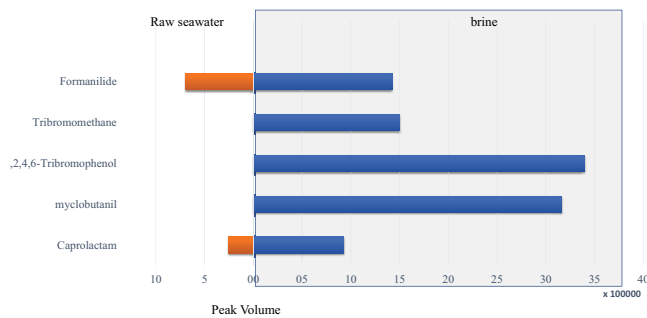


Fig. 5. Tentative new introduced contaminants.

Table 3
Results of peak comparison between raw seawater and brine

Spatial distance	Peak number	Ratio
0	496	31.8
<0.1	336	53.3
<0.2	202	66.3
<0.3	297	85.3
<0.4	100	91.7
<0.5	77	96.7
<0.6	23	98.1
<0.7	9	98.7
<0.8	9	99.3
<0.9	4	99.6
>0.9	7	100.0

desalination process increases its concentration above the detection limit. N-phenyl-formamide, and caprolactam are found in both seawater and brine. N-phenyl-formamide was mainly used for chemical synthesis and formerly as a local anaesthetic, analgesic, and antipyretic. Caprolactam

was used primarily in the manufacture of synthetic fiber. Their concentration in brine is about 2–3 times higher than in seawater. They may be from impurities of reverse osmosis scale inhibitors or released by membranes or pipelines.

4. Conclusion

For the first time, a combination of GC × GC-qMS and a QSAR model was successfully used to non-target identify and prioritize organic contaminants in raw seawater and desalination brine. Chromatographic peaks number, value and volume increase by 1.62%, 0.3%, and 3% after desalination, respectively. This gives a bird view of the different between brine and raw seawater for organic contaminants. A total of 55 compounds were tentatively identified, including two polycyclic aromatic hydrocarbons, three engineering plastic ingredients, nine pesticides, eight plasticizers, two disinfection by-products, four phosphate ester flame retardants, two chlorophenols, and 25 other industry intermediates. Among them, caprolactam, N-phenyl-formamide, 2,4,6-Tribromophenol and tribromomethane were probably introduced from the desalination process. PBT analysis showed that the contaminants identified in this study did not show high persistence and bioaccumulation. Some contaminants, for example, DEHP, show high toxicity to marine species. The influence of contaminants on different species is different. Therefore, the environmental effect of these contaminants may need to be confirmed in future studies. The method and results given in this study provide us with a new idea for identifying and prioritizing contaminants in desalination brine. They could help support the control of its environmental impact.

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Supporting information

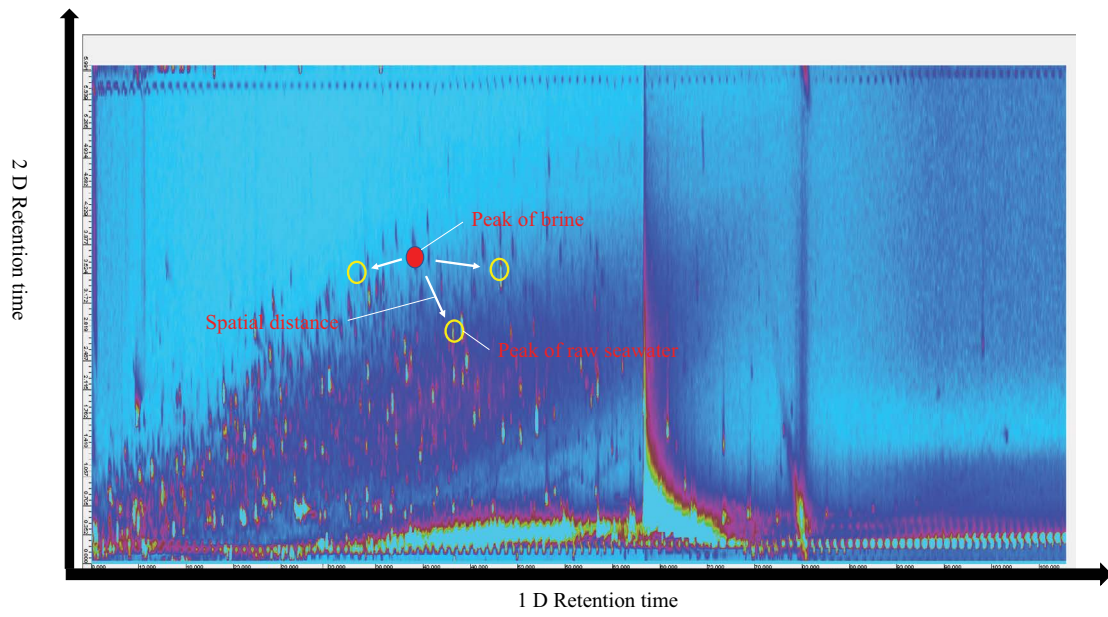


Fig. S1. Schematic diagram for new introduced chemical identification.