**Exsample: Screening of Chemical Structures Related to**

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**Haloacetic Acid Formation in Drinking Water Chlorination Process**

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**1． Introduction**

More than 200 compounds have been identified as disinfection by-products (DBPs) in actual tap water, and approximately 600 compounds are known as possible DBPs1). Among these compounds, haloacetic acids (HAAs) are one of the major groups of the DBPs, and its detection frequency and concentration are next to trihalomethanes (THMs) in finished drinking water2). Also, all of nine HAAs containing chlorine and bromine atoms are known to be toxic and some of them are suspected carcinogens3). Furthermore, brominated HAAs are more toxicic than their chlorinatd counterparts. Thus, it is important to understand the formation mechanism of HAAs in the presence of bromide ion to better control HHAs in drinking water treatment processes.

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However, despite the toxicological importance of HHAs, the formation mechanism of HAAs is not fully understood. This is mainly because of the complexity of the precursor of HAAs (i.e., dissolved organic matter (DOM)). DOM is a very complex mixture of organic compounds, and its structure is not clear, even today. To overcome this difficulty, the present study employs model compounds of DOM substructures. Similar approaches have been used for the studies on THM formation3,4), and successfully found the importance of *m*-dihydroxy structure for THM formation. However, no attempt has been made for HAA formation mechanism.

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**2． Experimental Methods**

**2．1　Material**

Model compounds of DOM substructures (Table 1) used in this study were purchased from Wako Pure Chemical unless otherwise noted. Their purity was more than 95% except lactic acid (85-92%) and used without further purification. Many of the model compounds were with carboxylic acids because carboxy group is one of the most common functional groups in DOM (Thurman, 1985). Also, phenolic compounds with different number of phenolic hydroxy groups were selected, as the number of phenolic hydroxy groups is an important factor of the susceptibility of aromatic rings to electrophilic substitution reaction. For aliphatic compounds, most of the selected compounds are carbohydrates, carboxylic acids, and carbonyl compounds. They were chosen based on the abundance in DOM structures5,6) and the susceptibility to the haloform reaction7).

**2．2 Analytical Methods**

HAA concentration was analyzed following USEPA method 552.39). Briefly, this method consists of liquid-liquid extraction, derivartization to haloacetate esters with acidic methanol, and GC-MS analysis (GC, Agilent 6890 with DB-5 column [J&W Scientific]; MS, JEOL JMS-AX505H).

**5． Conclusions**

In this study, HAA yields from 44 model compounds of DOM substructures were determined as a screening process of the chemical structures related to HAA formation. The major findings from this study are listed below:

* Phenolics (have higher HAA production than di-phenolic compounds.

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* When target compounds have high HAA production, they generate high amount of CHCl3, generally. Especially, correlations between these two productions are excellent in case of aliphatic compounds.
* Aromatic compounds tend to form larger amount of HAA (sum of HAAs) than aliphatic compounds. The former generally compose high amount of tri-HAA. The latter has greater di- and mono-HAA production.
* The presence of Br- made HAA production about 1.5 times higher than in absence of Br- for aromatic compounds. On the other hands, aliphatic compounds did not show this tendency.

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**References**

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**Key Words**: bromide ion, disinfection by products (DBPs), haloacetic acids, trihalomethanes