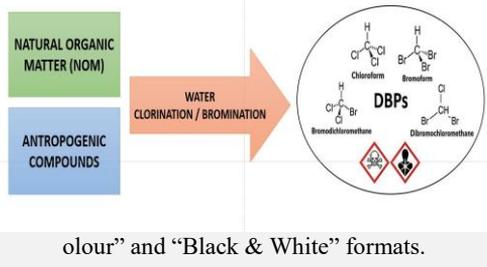


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Although being successfully applied all over the world water disinfection brings to formation of hazardous disinfection by-products (DBP) from natural and anthropogenic compounds always present in water. Over 700 DBP are known so far, being formed from natural humic matter. Every anthropogenic compound shows its unique scheme of transformation with formation of dozens and even hundreds DBP. Reactions of electrophilic substitution, electrophilic addition, nucleophilic substitution, oxidation, and even radical substitution result in a consecutive array of DBP, finishing with haloforms. Identification of novel DBPs and study of the mechanisms of their formation represents a challenging scientific task aiming improvement of human health and prevention of ecosystems pollution.

Aqueous chlorination of humic matter and numerous emerging contaminants (UV-filters, pharmaceuticals, cosmetic products) were studied with GC-HRMS and LC-HRMS. The reactions were carried out in laboratory in conditions close to that used at the water treatment stations. Besides, drinking water from several Russian cities and from swimming pools was analyzed to find DBP. The studies involved various disinfecting agents, variation of ratios, pH values, reaction time and temperature addition of inorganic salts. GC-MS experiments were performed using high resolution time-of-flight mass-spectrometers Pegasus GCxGC-HRT (LECO Corporation) and Orbitrap Exactive (Thermo

Scientific). LC-MS analyses were carried out with high-resolution TripleTOF 5600+ quadrupole time-of-flight (Q-TOF) (AB Sciex) and Orbitrap Tribrid (Thermo Scientific) mass spectrometers. Besides several low resolution GC-MS and LC-MS systems were used.

A number of novel DBPs including heterocyclic compounds and halogenated aliphatic amides were identified in the drinking water in terms of the study. Nevertheless, the most serious efforts were applied to the study of mechanisms of aquatic chlorination. Double bond appears to be more reactive in aqueous chlorination even than activated aromatic ring. Thus, primary reactions of active chlorine with resveratrol and avobenzon involve double bond, rather than aromatic ring. The presence of two double bonds in limonene allowed studying consecutive reactions of nucleophilic addition and elimination leading to a wide range of products with various number of chlorine atoms and hydroxyl groups. Although chlorination is usually conducted in the dark, radical reactions may still take place. Aqueous chlorination and bromination of benzalkonium chloride resulted in formation of numerous products with halogens in the aliphatic chain. On the contrary, aromatic ring remained unsubstituted. Aqueous chlorination of pharmaceutical doxazosin and arbidol demonstrated rather complex transformation including substitution, elimination, and oxidation processes. Bromides and iodides present in natural water form organohalogen species notably more toxic than the corresponding chlorinated ones. Long-term monitoring of volatile and semi volatile DBP in drinking water demonstrated fast penetration of bromine into the organic compounds at the initial stages of aqueous chlorination. Final DBPs (haloforms and haloacetic acids) contain much more chlorine than bromine due to higher content of chlorine in the reaction mixture and substitution of bromine for chlorine. The latter reaction (as well as substitution of iodine for chlorine) was studied on a wide raw of haloaromatic standards.

Acknowledgement

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