Identifying Toxic Compounds in Simulated Sewage-Treatment-Plant Effluents by a Non-Targeted Mass Spectrometric Analysis and the Whole Effluent Toxicity Test.

Atsushi SAWAI*, **, Tetsuro OKAMURA*, Nobukazu MIYAMOTO*, Yuta SHINFUKU**, Hirokazu TAKANASHI**

*Institute of Environmental Ecology, IDEA Consultants, Inc., Shizuoka 421-0212 Japan
**Graduate School of Science and Engineering, Kagoshima University, Kagoshima 890-0065 Japan

Simulated samples of sewage-treatment-plant (STP) effluent were prepared by adding five known toxic compounds to the actual STP effluents. The name of the added compound was concealed to the analyst. The exploration and identification of toxic compounds in the samples were conducted by coupling a non-targeted mass spectrometric analysis with the whole effluent toxicity (WET) test. The number of detected components with a high resolution mass spectrometer (Acquity H-Class-Synapt G2-Si, Waters, MA, USA) was 3,427. The orthogonal projections to latent structures and correlation analysis were performed on the test results, narrowing down the number of candidates. One dominant candidate was focused as a result of multiple regression analysis (stepwise selection method). Accurate mass spectrum of the candidate was obtained with another high resolution mass spectrometer (UltiMate HPG-3400SD-LTQ Orbitrap XL, Thermo Scientific, MA, USA) to elucidate its molecular formula. It was successfully identified as triclosan by database matching and co-chromatography with an authentic standard chemical reagent. Other toxicants added to the samples were confirmed to be negligible to the total toxicity of the samples. These results demonstrated the effectiveness of the presented methodology.