Suspect and non-target screening of emerging contaminants in wastewater using LC-QTOF/MS: An insight on occurrence, fate, risk, and wastewater management in Asia

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Introduction

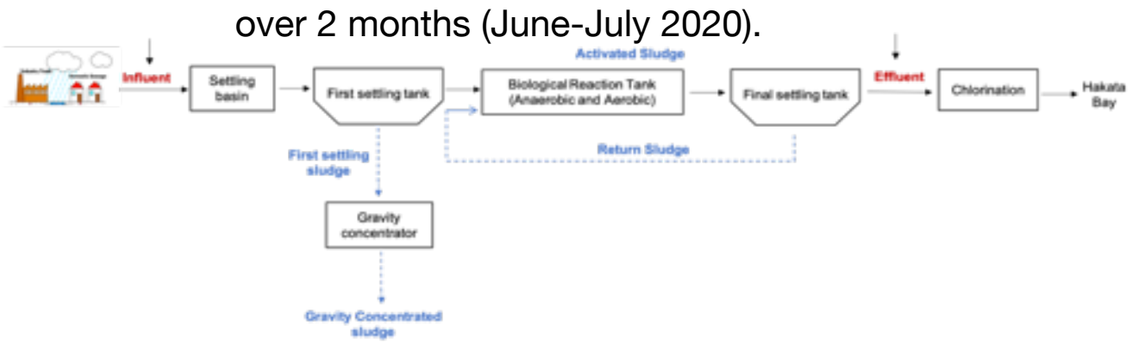
- Domestic wastewater is a major pollution source to water environment in many **Asian countries**. In the respect of water environmental conservation, it is important to reduce the pollution load from domestic sector.
- Understanding of sate of water quality through identification of pollution source is the first step in establishing an ambient water quality standard.
- Suspect and non-target analysis are part of a systematic screening strategy for contaminants.

- The aim is to develop a comprehensive workflow for suspect and non-target screening using LC-Q-TOF/MS for identifying different contaminants, study their fate and assess their toxicity risk.
- **The workflow would have wider implication in wastewater management in Asia region.**

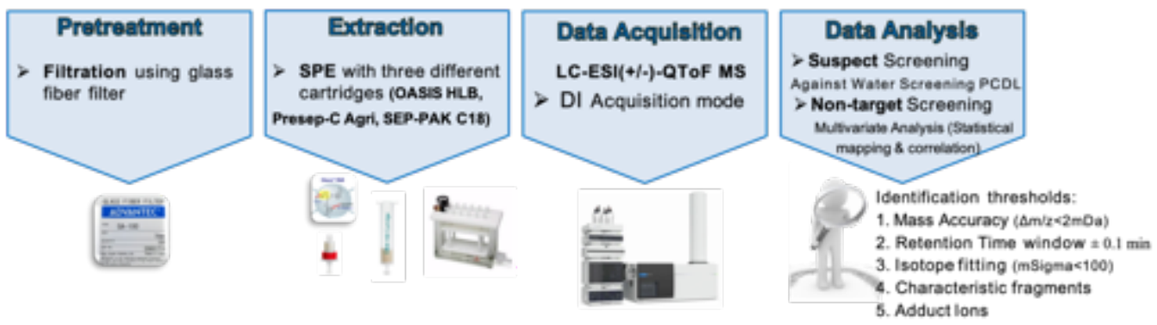
Methodology Workflow

Sampling

- Influent and effluent of wastewater treatment plant (WWTP) in Fukuoka city were sampled Once a week over 2 months (June-July 2020).



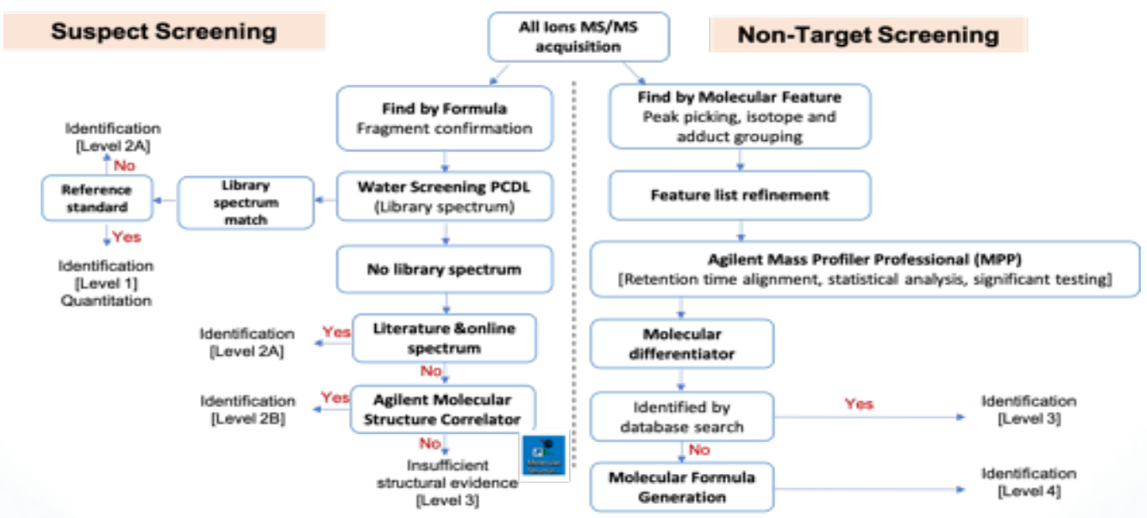
Analysis Workflow



Data Acquisition

- Zorbax SB-C18 column (15.0 cm × 0.21 cm, 3.5 µm).
- Mobile phase A: 5 mM Ammonium formate + 0.1% FA in H2O, and B: 0.1% FA in ACN at a flow rate of 0.4 mL/min
- Accurate mass spectra were acquired in (ESI) in All Ions MS/MS acquisition with 4 scans/sec with four discrete collision energies (one full scan at 0 eV, followed by MS/MS scan at 10, 20, 40 V).

Workflow for Data Analysis



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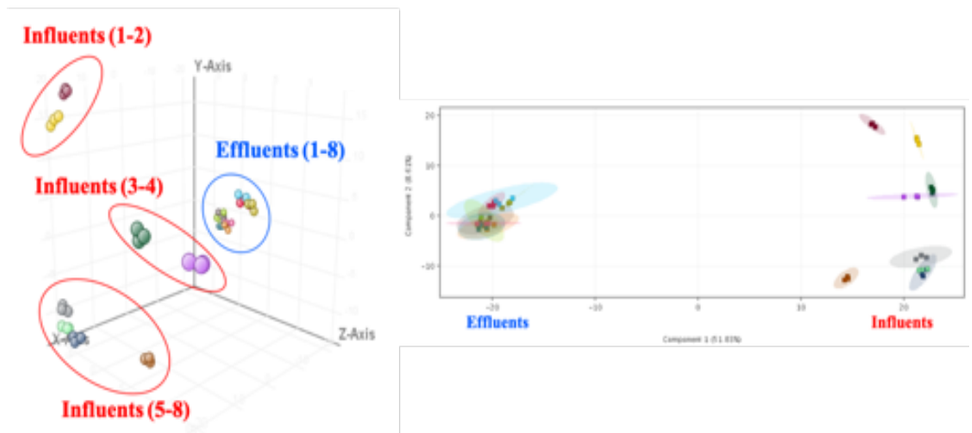
Results

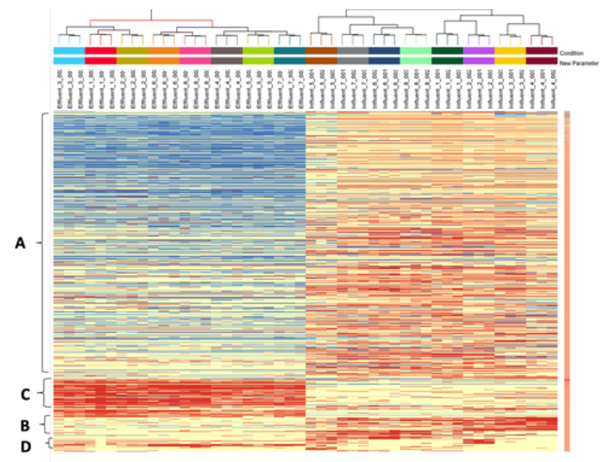
Multivariate Analysis

- PCA plots represent a significant differentiation between sample groups demonstrating an **effective WWTP treatment process**.

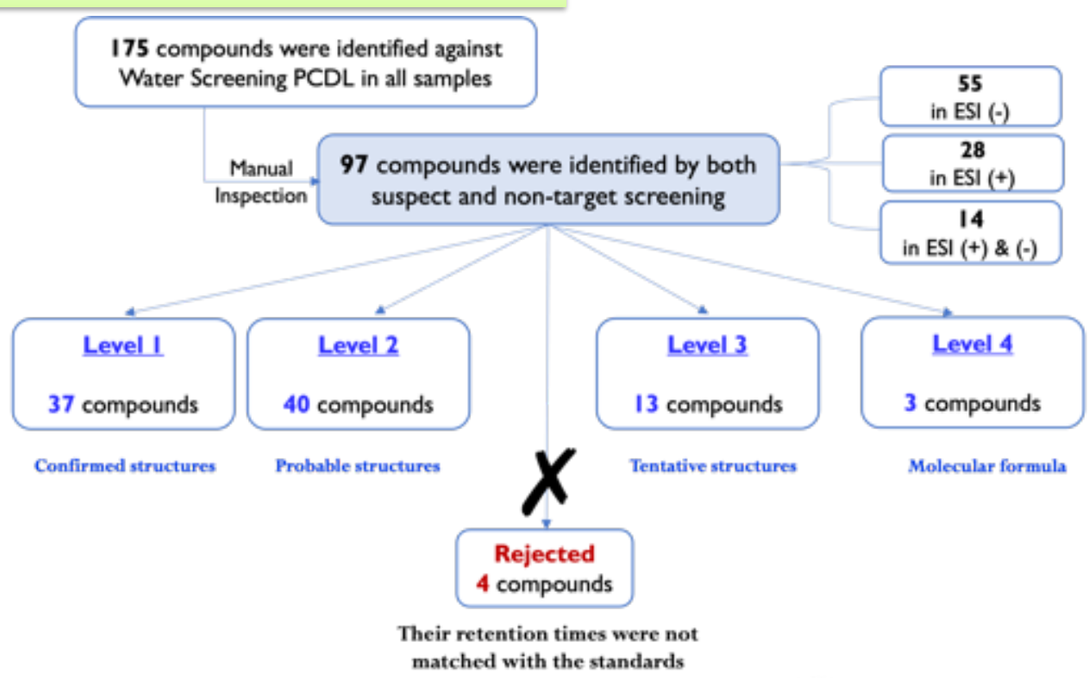


- HCA revealed **several groups of compounds that differed in their response to treatment**:

I. Compounds **removed** by treatment (**A & B**).
II. Compounds **formed** during treatment (**C**).
III. Compounds **resistant to** treatment (**D**).

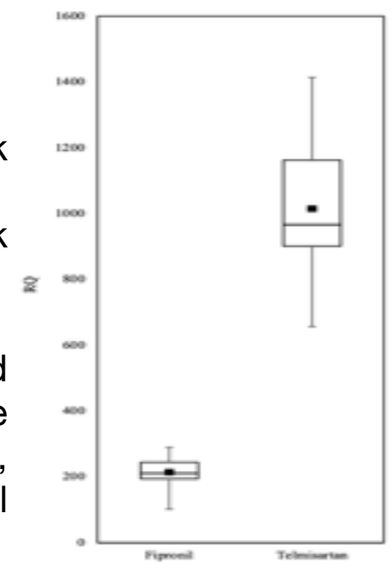


Compounds Identification



Toxicity and Risk Assessment

- Most of compounds showed either low risk (RQ < 0.1) or medium risk (0.1< RQ <1).
- **Telmisartan** and **fipronil** showed high risk to aquatic organisms (RQ > 1).
- **The low PNEC values** (0.00055 and 0.00077 µg/L) are mainly responsible for the high RQ of **telmisartan** and **fipronil**, respectively, demonstrating their potential toxicity at ecologically relevant amounts.



Conclusion

- The occurrence of contaminants in WWTP was investigated by suspect and non-target analysis using LC-QTOF/MS. Compounds from different classes were identified at different confidence levels.
- Telmisartan and fipronil are considered with more environmental significance (RQ > 1).
- Multivariate analysis demonstrated a significant differentiation between sample groups confirming an effective wastewater treatment process.
- **The results of this work could be reflected in future water quality monitoring plans in Asian developing countries.**