Paper presentation

Atrayee Datta
22nd June 2024

Environmental Science & Technology

pubs.acs.org/est

Article

Target and Nontarget Screening to Support Capacity Scaling for Substance Use Assessment through a Statewide Wastewater Surveillance Network in New York

Emily J. Vogel, Milagros Neyra, David A. Larsen, and Teng Zeng*

Publication date: 1st May 2024

Corresponding Author

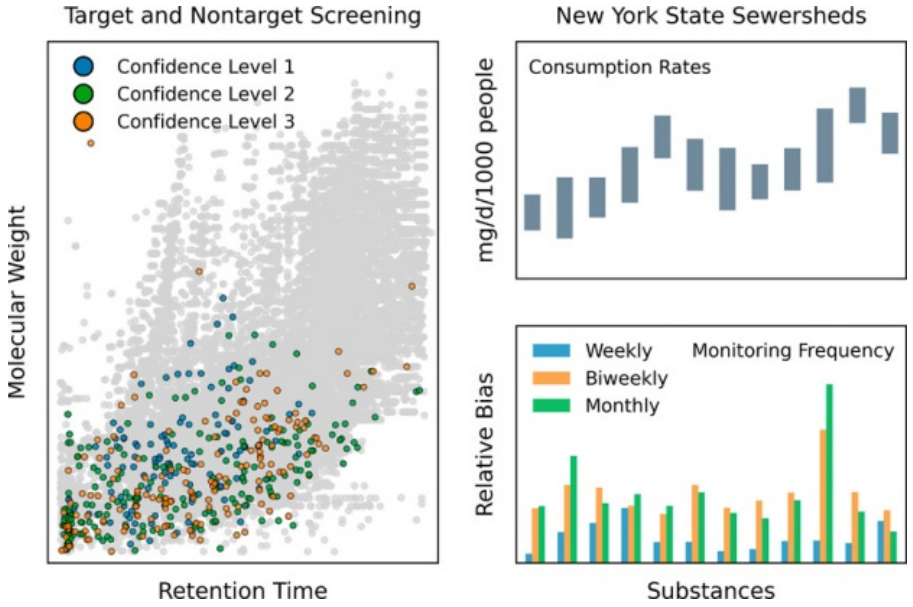
Teng Zeng – *Department of Civil and Environmental Engineering, Syracuse University, Syracuse, New York 13244, United States;* orcid.org/0000-0002-0374-9549; Phone: +1-315-443-1099; Email: tezeng@syr.edu

Authors

Emily J. Vogel – *Department of Civil and Environmental Engineering, Syracuse University, Syracuse, New York 13244, United States*

Milagros Neyra – *Department of Public Health, Syracuse University, Syracuse, New York 13244, United States*

David A. Larsen – *Department of Public Health, Syracuse University, Syracuse, New York 13244, United States*



Terminologies

- ✓ **Psychoactive substances:** Substances that are taken in or administered into one's system, affect mental processes, example perception, consciousness, cognition or mood and emotions.

- ✓ **Substance use assessment:** Substance use assessment are critical tools used by professionals to evaluate an individual's or population's substance abuse, identify potential substance use disorders (SUDs), and guide appropriate treatment plans.

- ✓ **Target screening:** Target screening of wastewater involves the analysis of water samples to detect or quantify specific contaminants or compounds of interest.

- ✓ **Non-target screening:** Non-target screening of wastewater is a powerful approach to understanding the complex and dynamic nature of wastewater composition, enabling the detection of both known and unknown contaminants.

Background

Wastewater analysis and drugs — a European multi-city study

Water Research X
Volume 19, 1 May 2023, 100179

Journal of Hazardous Materials
Volume 384, 15 February 2020, 121306

Three years of wastewater surveillance for new psychoactive substances from 16 countries

Prevalence of illicit and prescribed neuropsychiatric drugs in three communities in Kentucky using wastewater-based epidemiology and Monte Carlo simulation for the estimation of associated uncertainties

Environmental Science & Technology
pubs.acs.org/est
Article

Occurrence and Mass Loading of Synthetic Opioids, Synthetic Cathinones, and Synthetic Cannabinoids in Wastewater Treatment Plants in Four U.S. Communities

Catherine E. O'Rourke and Bikram Subedi*

Objective

Explore the operational feasibility keeping in mind the growing capacity of WBE for substance use assessment in the US

Develop an integrated analytical framework for routine, accurate and fast quantification of most frequently detected target substances.

Qualitative screening of non- targeted analogues, their derivatives, and emerging substances of concern. This includes new psychoactive substances.

Method of study

- ✓ Sampling: 24 hour composite influent samples were collected from 10 Wastewater Treatment Plants (WWTPs) at mixed intervals over multiple months between 2021 and 2022.
- ✓ Samples were transported overnight and stored at -80°C.
- ✓ Wastewater samples were spiked with a mixture of 42 isotopically labeled internal standards (ILIS)
- ✓ Further, they were analyzed using online solid phase extraction (SPE) system coupled with liquid chromatography-high resolution mass spectrometry (LC-HRMS).

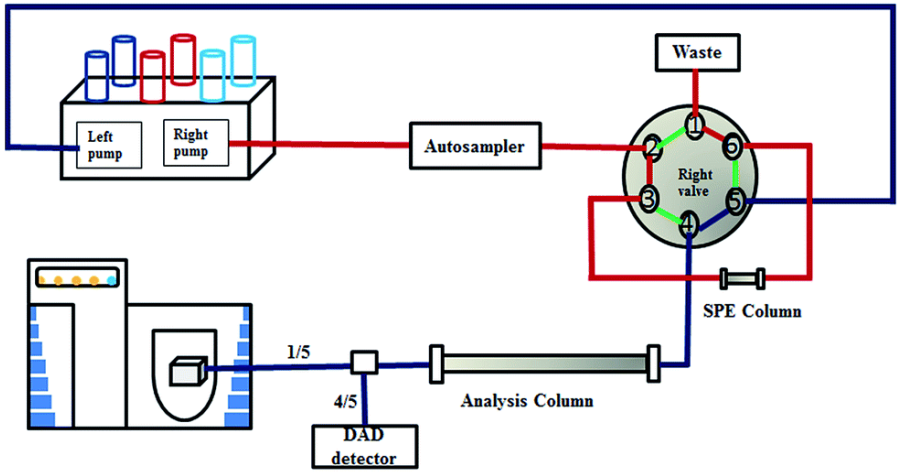


Fig: Schematic of online SPE coupled with LC- HRMS

- ✓ Calibration standards of target substances was run with each sample sequence.
- ✓ Continuous blanks were run every ten samples to prevent drift in instrument performance and minimize carryover.

Target screening

- ✓ Target substances were confirmed by verifying their retention times and dd-MS2 spectra against those of reference standards.
- ✓ Calibration curves for target substances were generated by linear or quadratic regression.
- ✓ Unknown concentration was obtained from the calibration curves.
- ✓ The population normalized mass loads (PNMLs) and consumption rates (CRs) were back-calculated using drug target residues (DTRs):

$$PNML_{i,j} = C_i \times Q_j \times \left(\frac{100}{(100 + stability_i)}\right) \times \left(\frac{100}{(100 - sorption_i}\right) \times \left(\frac{1000}{population_j}\right)$$

$$CR_{i,j} = PNML_{i,j} \times \left(\frac{1}{excretion_i}\right) \times \left(\frac{MW_{i,parent}}{MW_{i,DTR}}\right)$$

'*i*' is the substance and '*j*' is the treatment plant.

Results

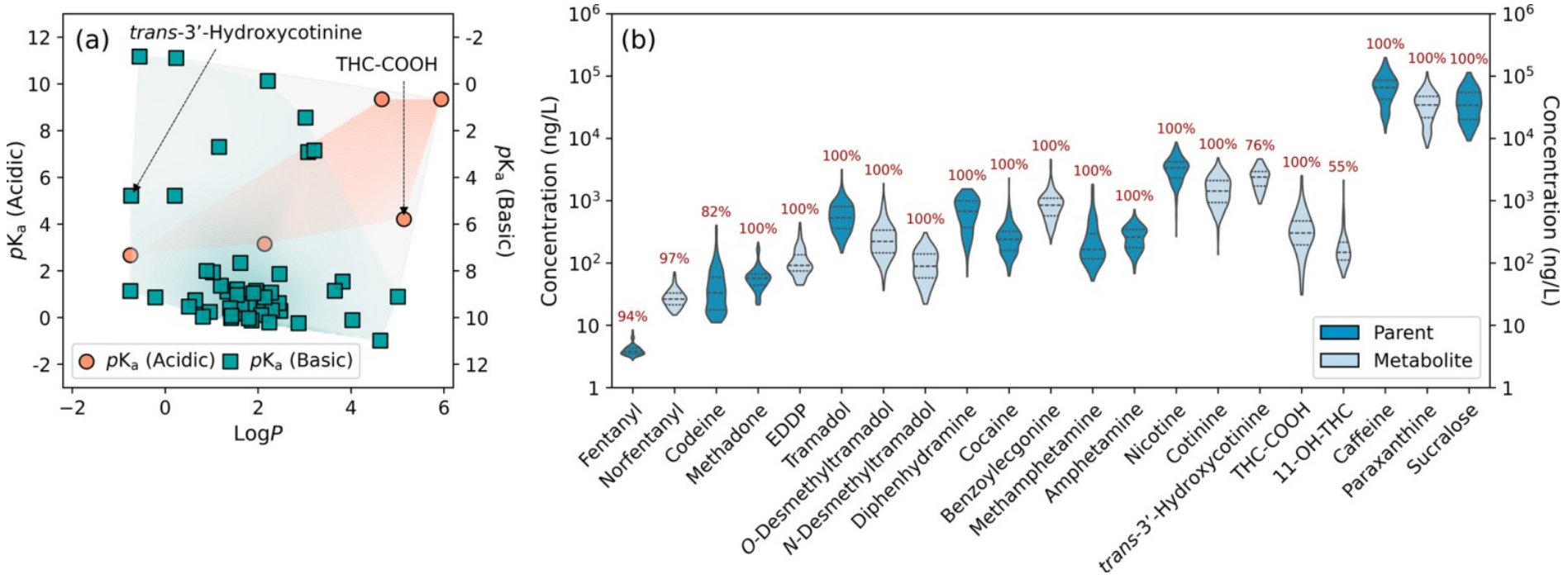


Fig: (a) Target substances (n = 51) validated by the online SPE-LC-HRMS method developed in this work.

(b) Target substances (n = 21) detected in over 50% of wastewater samples.

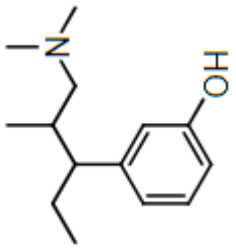
Non-target screening

Non- target screening was done at 3 confidence levels:

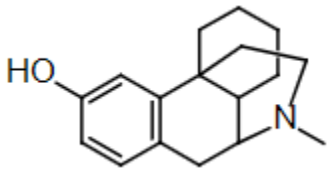
i. Confidence level 1: 86 compounds were confirmed at level 1 by reference standards
ii. Confidence level 2: 196 were identified at level 2 as probable structures by library matching
iii. Confidence level 3: 158 assigned as tentative structures by diagnostic fragments and neutral losses

Compounds prioritized by non-target screening were confirmed psychoactive substances with abuse potential.

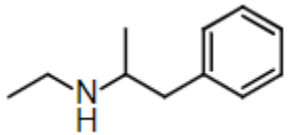
Confidence level 1



Tapentadol

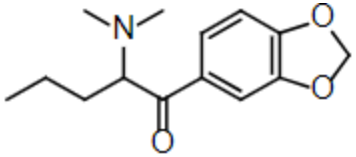


Levorphenol

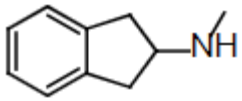


N-Ethylamphetamine

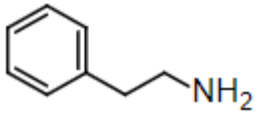
Confidence level 2



N,N-dimethylpentylone

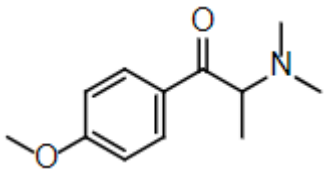


N-methyl-2-aminoindane

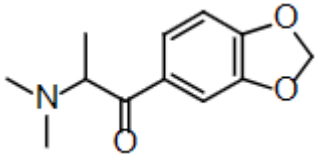


2-phenethylamine

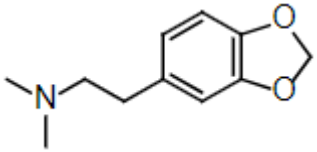
Confidence level 3



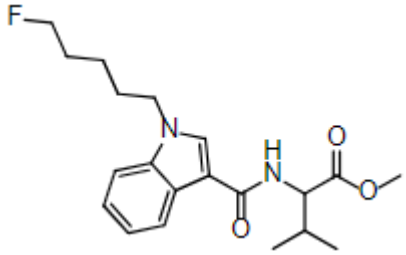
4-methoxy-N,N-dimethylcathinone



Dimethylone



N-methyl homarylamine



5-fluoro AMB-PICA

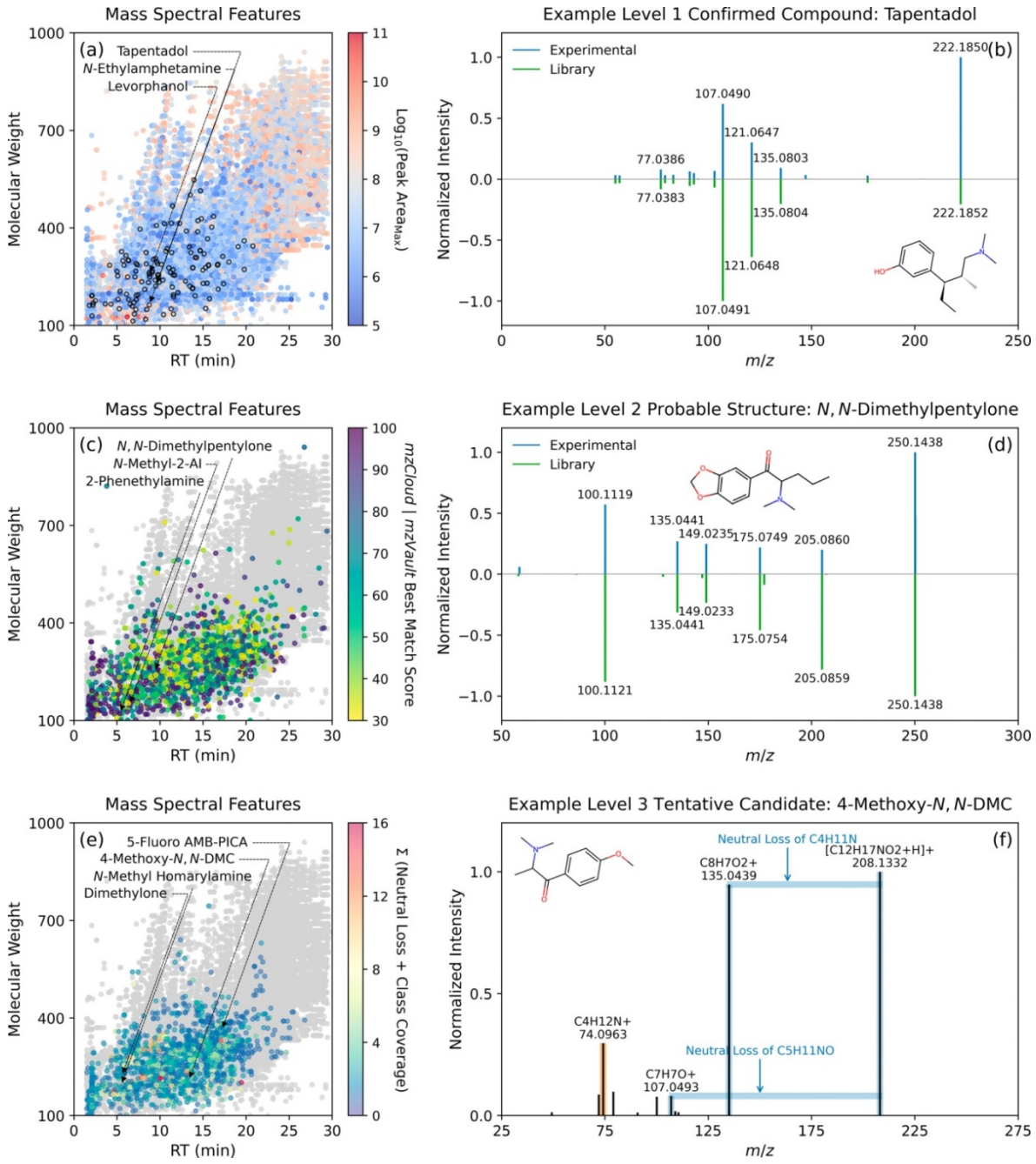


Fig: Non-target screening of substances in wastewater samples

Consumption estimates of target substances

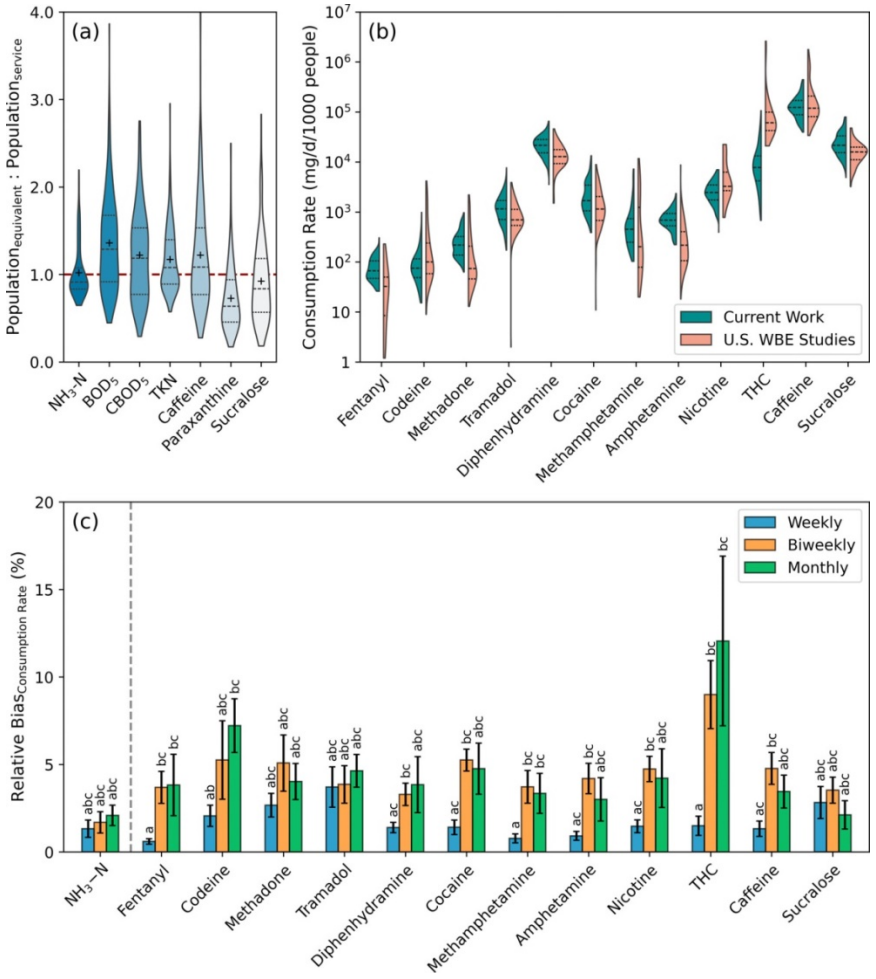


Fig: (a) Comparison of sewershed populations with service population
(b) Consumption rates of substances (in mg/day/1000 people) estimated in this work compared with those reported by 15 WBE studies conducted in the U.S. between 2014 and 2024 (c) Effect of monitoring frequency on relative bias in consumption rates

Parent to metabolite ratios

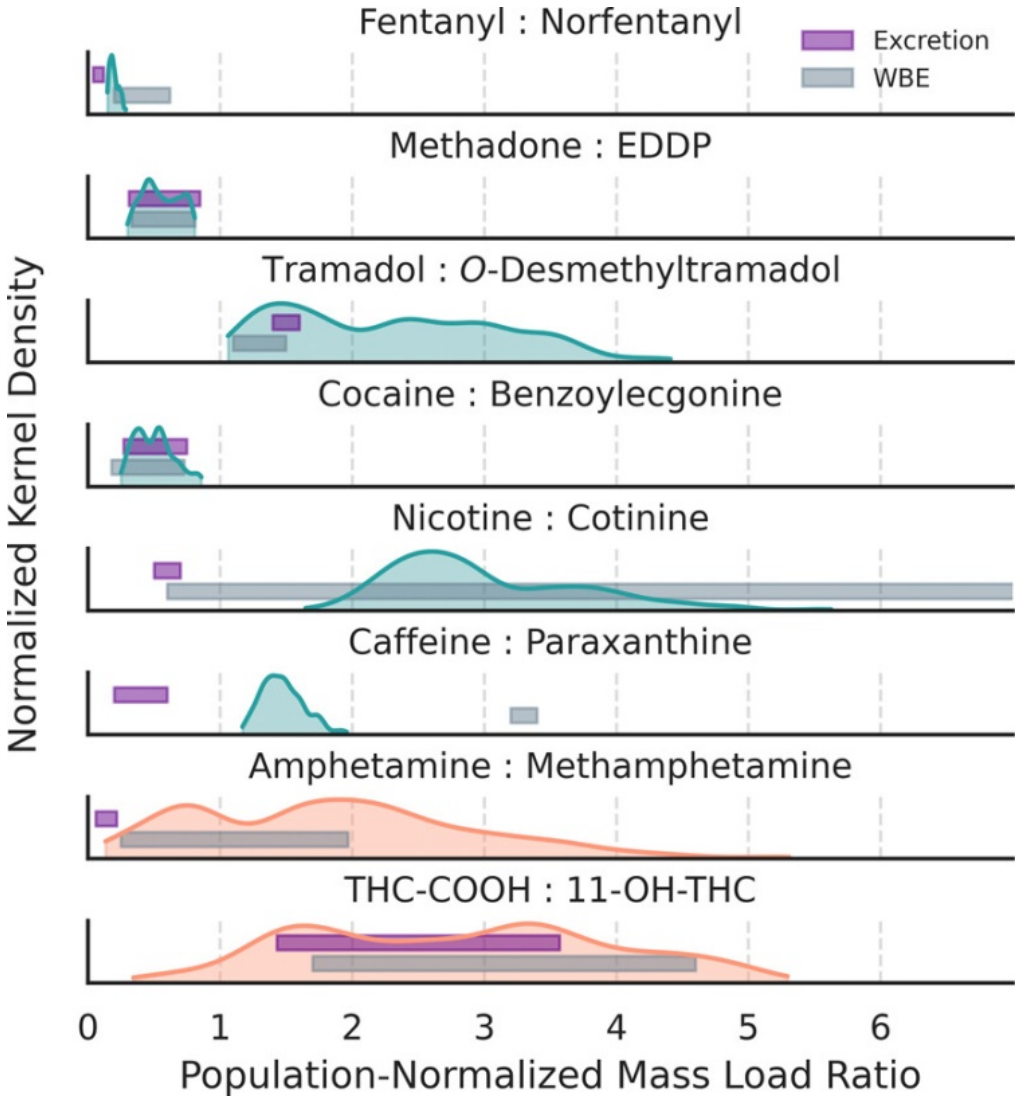


Fig: Comparison of population-normalized mass load (PNML) ratios for structurally related target substances

Conclusions

- ✓ This paper highlights the potential of wastewater-based epidemiology (WBE) as an effective monitoring tool
- ✓ The work demonstrated the potential of online SPE-LC-HRMS for high throughput quantification and non-target analysis.
- ✓ Target screening covered a range of acidic, lipophilic, and basic hydrophilic compounds
- ✓ Non-target screening covered wide range of psychoactive substances reported in previous WBE studies.

Limitations

- ✓ Consumption estimates relied on back calculations that were highly sensitive to uncertainties
- ✓ And generating such estimates would be impractical for substances without known metabolic pathways and excretion rates, or not excreted in detectable quantities