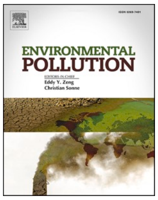
Environmental Pollution 397 (2026) 127930

Contents lists available at ScienceDirect

Environmental Pollution

journal homepage: www.elsevier.com/locate/envpol



In situ evaluation of an active-passive sampling (APS) technique for monitoring psychoactive compounds in effluent wastewater

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ARTICLE INFO

Keywords:
Wastewater monitoring
Active-passive sampling (APS)
Diffusive gradients in thin films (DGT)
Psychoactive compounds
Uptake kinetics
Predictive modelling

ABSTRACT

Monitoring of psychoactive drugs and their metabolites in wastewater is critical to understanding their environmental fate and potential impacts. Passive sampling offers a complementary approach to conventional composite sampling, providing time-integrated monitoring, while offering insights into bioavailable fractions of compounds. This study evaluates the applicability of an active-passive sampling (APS) approach for monitoring eight psychoactive compounds in effluent wastewater, integrating field deployments with predictive modelling of sorbent-to-water partition coefficients (K_{SW}). APS and diffusive gradients in thin films (DGT) samplers, equipped with hydrophilic-lipophilic balanced (HLB) and mixed-mode cation exchange (MCX) sorbents were deployed alongside daily composite sampling during 2023-2024 monitoring campaigns in Belgium and Slovenia. APS exhibited non-linear uptake kinetics indicative of non-ideal sink behaviour and additional mass-transfer limitations, including interfacial effects, while DGT uptake remained predominantly diffusion-controlled over the deployment periods. K_{SW} values were predicted using tree-based machine-learning models (Random Forest and XGBoost), enabling robust interpretation of APS data under near-equilibrium conditions. APS and DGT measurements generally showed good agreement, though APS concentrations were systematically higher for most compounds, with differences influenced by sorbent type and environmental factors. The controlled laminar flow of APS enhanced sorption consistency under variable wastewater conditions. Comparisons with composite sampling highlighted the complementary nature of these approaches, with APS providing additional insights on bioavailable and particle-bound fractions. Overall, APS presents a robust and versatile tool for monitoring psychoactive compounds, supporting quantitative assessment of contaminant dynamics, bioavailability, and fate in aquatic systems.

1. Introduction

Psychoactive compounds, including legally prescribed medications and illicit drugs, are increasingly detected in urban wastewater worldwide, raising environmental concerns due to their persistence and ineffective removal during wastewater treatment (Jin et al., 2022; Salgueiro-Gonzalez et al., 2024). Wastewater analysis of psychoactive compounds has been widely utilised to assess their occurrence, fate, and potential ecological risks (Jin et al., 2022; Semerjian et al., 2018; Wang et al., 2023). The general procedure involves collection of daily composite wastewater samples, followed by chemical analysis to detect and quantify target compounds or their metabolites (Perspectives on Drugs, 2025; Sulej-Suchomska et al., 2020). In wastewater monitoring protocols, the sampling method remains a critical factor influencing data quality and reliability as it directly affects uncertainties in estimating aqueous concentrations (Castiglioni et al., 2013; Singer et al., 2023). Composite sampling is commonly used to capture temporal fluctuations but it can be logistically demanding, and transient concentration spikes may not be captured depending on the sampling mode (time- or flow-proportional) and sampling intervals (Ort et al., 2010;

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https://doi.org/10.1016/j.envpol.2026.127930
Received 23 January 2026; Received in revised form 4 March 2026; Accepted 5 March 2026
Available online 10 March 2026
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Shakallis et al., 2022). As such, the sampling strategy must be carefully evaluated taking into account practicality, sensitivity, and temporal resolution, especially when monitoring low-abundance or labile psychoactive compounds.

A complementary approach that addresses these challenges is passive sampling (PS), which has emerged as a valuable tool for monitoring psychoactive compounds and other pharmaceuticals. Passive samplers, such as diffusive gradients in thin films (DGT), Chemcatcher™, polar organic chemical integrative samplers (POCIS), and microporous polyethylene tubes (MPT), provide in situ preconcentration of target analytes and subsequent estimation of time-weighted average (TWA) concentrations. These concentrations also reflect the freely dissolved fraction of analytes in water, which is bioavailable to organisms and therefore critical for evaluating environmental exposure (Godlewska et al., 2021; Shakallis et al., 2022). However, challenges remain regarding the robustness of PS measurements, as environmental factors significantly affect the uptake of analytes by PS devices. For instance, variations in water temperature, flow velocity, turbulence, and biofouling of the sampler surfaces can alter uptake kinetics (Becker et al., 2024; Booij et al., 2016), while changes in pH, dissolved organic matter, and suspended solids may affect the proportion of the analytes that exist in freely dissolved form (Anies et al., 2025; Petrie et al., 2015).

In this study, we applied the active-passive sampling (APS) strategy to monitor psychoactive compounds in effluent wastewater. APS is an innovative sampling technique capable of simultaneously determining the concentrations of inorganic and organic (polar and nonpolar) analytes in aquatic environments. Unlike standard passive samplers, APS incorporates both active and passive sampling wherein the sampled medium is actively pumped through a diffusion cell containing different receiving phases (sorbents) that accumulate the target analytes. Importantly, the APS device incorporates an internal pump to regulate the flow through the sampler and a flow meter to regularly measure and record the flow rate. The controlled laminar flow feature of the APS enables measurements that are independent from the hydrodynamic conditions of the bulk medium, and thereby reducing uncertainties related to flow variations and overcoming limitations associated with conventional passive sampling techniques (Amato et al., 2021, 2018).

The interpretation of APS and other passive sampling data depends on whether uptake occurs in the kinetic or equilibrium regime. Sampling rates (R_S) are used to quantify concentrations under kinetic conditions, while sorbent-water partition coefficients (K_{SW}) become critical when samplers operate under equilibrium or near-equilibrium. However, both parameters are compound-specific and highly dependent to environmental variables such as pH, ionic strength, temperature, and water flow conditions (Amato et al., 2021; Becker et al., 2024; Godlewska et al., 2021).

This study focused on monitoring eight target psychoactive compounds (amphetamine, benzoylecgonine, EDDP, hydroxybupropion, morphine, O-desmethylvenlafaxine, tramadol, and trazodone) and assessed the APS performance in comparison with conventional composite sampling and passive sampling by DGT. The field-based evaluation of APS was conducted across three sampling campaigns on effluent wastewater in two countries (Belgium and Slovenia), providing insights into uptake kinetics, repeatability of measurements, and inter-method comparability. To augment the interpretability of APS under near-equilibrium conditions, we applied machine-learning approaches (XGBoost and Random Forest) to predictive modelling of compound-sorbent conditional K_{SW} values using laboratory data obtained under varying environmental conditions (pH, ionic strength, and temperature). This integrated approach addresses key challenges in wastewater analysis by combining novel in situ sampling, robust analytical workflows, and predictive modelling to improve monitoring of psychoactive compounds in wastewater environments.

2. Materials and methods

2.1. Target analytes and chemicals

Eight psychoactive compounds (amphetamine, benzoylecgonine, EDDP, hydroxybupropion, morphine, O-desmethylvenlafaxine, tramadol, and trazodone) were selected based on existing analytical protocols and their frequent occurrence in previous monitoring campaigns. The selection consists of parent compounds or primary metabolites of antidepressants, opioids, and illicit drugs. Physicochemical properties, chemical structures and speciation at average wastewater pH (7.0-8.0) are presented in the Supplementary Information (Fig. S1A).

Reference standards and deuterated internal standards (IS) of the target compounds were obtained from Cerilliant Corp. (USA), LGC Standards (UK), and Toronto Research Chemicals (CA). Stock and working solutions of the standards were prepared in methanol and stored at −20 °C. Other analytical-grade solvents and chemicals were purchased from various reputable suppliers.

2.2. Active-passive sampling (APS) device and sorbents

A diagram of the APS device is shown in Fig. S2. The APS device features a diffusion cell, a pump on the inlet and a flow meter on the outlet to regulate a constant flow-through system, and temperature and humidity sensors (Fig. S2b). Regular measurements of flow rate (set at 5.4 $cm^3\ s^{-1}$), water (inlet and outlet) and air temperature are logged using a cloud-based monitoring application. An example of a read-out of measurements is provided in Fig. S3. The diffusion cell consists of two blocks of polyether ether ketone (PEEK) with a 5 mm thick spacer (Amato et al., 2021, 2018). Each block contains pockets designed to house the receiving phases of 40 × 20 mm and 20 × 20 mm sizes per sorbent.

HLB (hydrophilic-lipophilic balanced) and MCX (mixed-mode cation exchange) were selected to capture a broad range of psychoactive compounds differing in polarity and ionization state (Boogaerts et al., 2023, 2021; Laimou-Geraniou et al., 2025) (Fig. S1A). HLB enables retention of both polar and moderately nonpolar analytes through hydrophilic and reversed-phase interactions, whereas MCX provides additional selectivity for positively charged compounds via strong cation-exchange mechanisms (Bäuerlein et al., 2012) (Fig. S1B). These features allow efficient extraction of neutral, polar, and ionizable species commonly encountered among psychoactive compounds and their metabolites. HLB and MCX polymeric sorbents purchased from Affinisep (FR) as custom-made AttractSPE™ pads, with 90% w/w sorbent material and a thickness of 0.5 mm, were used as receiving phases for the APS device. The sorbents were conditioned with methanol and deionised water prior to assembly of the diffusion cell, and each receiving phase was topped with a filter membrane (polyethersulfone, PES, 0.2 μm pore size, 145 μm thickness). The APS device was externally connected to a filter (100 μm nylon mesh) to prevent the entry of large particles into the diffusion cell.

2.3. Organic diffusive gradients in thin films (o-DGT)

The o-DGT samplers used in the sampling campaigns were constructed based on the standard DGT configuration with the same receiving phases as those used in the APS device (exposed area = 3.14 cm^2, thickness = 0.5 mm). The HLB- and MCX-based binding layers were topped with an agarose diffusive gel (1.5% w/w, 0.75 mm thickness) and a PES filter membrane (0.2 μm pore size, 145 μm thickness). For comparison, commercially available o-DGT samplers with an HLB binding gel, a 0.8 mm agarose diffusive gel, and a PTFE filter membrane were purchased from DGT® Research (UK).

2.4. Field study design

Field sampling campaigns were conducted at a wastewater treatment plant (WWTP) in Aartselaar, Belgium (summer 2023 and 2024), and the Ljubljana Central WWTP in Slovenia (autumn 2023). Both facilities operate conventional activated sludge processes with biological nitrification-denitrification and secondary clarification, but differ widely in treatment capacity and influent composition. Aartselaar WWTP mainly receives residential wastewater with an approximate population size of ~65,000, while Ljubljana WWTP treats mixed domestic and industrial wastewater (population equivalent ~360,000).

The APS and DGT samplers were deployed in the effluent wastewater concurrently at five staggered time points over a sampling duration of up to 14 days (Table S3A), depending on the WWTP constraints. At each time point, one APS device (containing duplicate HLB and MCX sorbents) and three DGT samplers per sorbent type were installed. In the 2024 sampling campaign, the deployment period was limited to a maximum of seven days due to operational restrictions. The staggered and occasionally overlapping deployments were designed to generate accumulation profiles for calibration purposes. In addition, the repeatability of APS and DGT was evaluated during the 2024 campaign by deploying three replicate APS devices alongside corresponding DGT samplers over a six-day sampling period.

Samplers were retrieved at each interval and daily effluent samples were collected using 24-h time-proportional automatic composite samplers installed by the WWTPs. Sorbents and water samples were stored at −20 °C until further analysis. Sampling dates, and water quality parameters are documented in *S3*.

2.5. Sample preparation and instrumental analysis

Exposed and unexposed (blank) APS and DGT sorbents from all sampling campaigns were extracted following the procedure reported by Anies et al. (2025) using a total extraction volume of 8 mL. HLB sorbents were extracted with 2% formic acid in methanol whereas MCX sorbents were extracted with 1.25% NH_3 in methanol. Composite effluent samples from Belgium were extracted using 96-well SPE following the protocol reported by Boogaerts et al. (2023), and those from Slovenia by off-line SPE following a modified procedure reported by Laimou-Geraniou et al. (2025), with both methods using MCX sorbent. Oasis MCX 96-well plates (30 μm, 10 mg) and Oasis Prime MCX 6 cc cartridges (30 μm, 150 mg) were purchased from Waters™ (USA). The Belgian samples (APS, DGT, and 24-h composite effluent wastewater extracts) were analysed by liquid chromatography-tandem mass spectrometry (LC-MS/MS) and the Slovenian samples by gas chromatography-tandem mass spectrometry (GC-MS/MS). Detailed extraction and quantification protocols are provided in *S4*.

2.6. Uptake kinetics of passive samplers and c_W calculations

For each analyte, the uptake profile over time was assessed to determine whether the accumulation followed the linear or curvilinear regimes. These temporal profiles were used to construct calibration curves and estimate time-weighted average (TWA) concentrations.

Assuming a steady-state diffusion in the aqueous medium, the concentration of compound X in the sorbent phase, $c_{S,X}$ (nmol L^{-1}), evolves exponentially through time (t),

$$c_{S,X} = c_{w,X} K_{SW,X} \left(1 - exp^{-k_X t}\right) \tag{1}$$

where $c_{W,X}$ (nmol L^{-1}) is the concentration of X in the water phase, $K_{SW,X}$ (dimensionless) is the sorbent-water partition coefficient of X, and k_X (h^{-1}) is the accumulation rate constant. In the linear regime, uptake is governed by the diffusive flux of the analyte from the water phase to the sorbent phase. Following Fick's first law of diffusion and the description of flux as a function of time, $c_{S,X}$ can be expressed by:

$$c_{S,X} = c_{W,X} D_X A_S t / V_S \delta \tag{2}$$

where D_X ($m^2 s^{-1}$) is the diffusion coefficient of X, A_S (m^2) and V_S (m^3) are the exposed surface area and volume of the sorbent, respectively, and δ (m) is the thickness of the diffusion layer (Zhang and Davison, 1995). For APS, δ was estimated using the flow rate within the diffusion cell and the position of the receiving phase in the diffusion channel (Amato et al., 2018). For DGT, mass transfer is regulated by the agarose diffusive gel, thus, δ was assumed to be the thickness of the diffusive gel layer, (Δg). D_X values for each compound were previously determined and conversions at different temperatures were done according to the equation reported by Zhang and Davison (1995) (Eq. S(3) in the Supplementary Information).

2.7. Predictive modelling of conditional K_{SW}

To estimate the K_{SW} of the compounds under various environmental conditions, a set of models was developed using previous experimental data (Anies et al., 2025). To capture both mechanistic trends and data-driven non-linearities in K_{SW}, three modelling approaches were employed: (i) Bayesian linear regression, which quantifies probabilistic relationships while explicitly accounting for uncertainty; (ii) Random Forest, an ensemble of decision trees that captures non-linear responses and higher order interactions through bootstrap aggregation; and (iii) XGBoost, a gradient-boosted tree algorithm optimized for learning structured non-linear relationships and complex feature interactions. These models were applied for the measured $K_{SW,X}$ values across a range of water parameters (pH, conductivity, and temperature).

Models were trained separately for each compound and sorbent combination in R (version 4.3.1) via RStudio, using *bayesreg* (Makalic and Schmidt, 2016), *randomForest* (Liaw and Wiener, 2002), and *xgboost* (Chen and Guestrin, 2016) packages. Experimental data were used as input, with environmental parameters serving as predictors. Features were transformed using logarithmic ($\log_{10}$) and polynomial (x^2) terms, and interaction terms (e.g., pH × Temperature, pH × Conductivity). Datasets were split 80:20 into training and test sets and random seeds were set independently for each compound-model combination to ensure reproducibility. Hyperparameters were optimized via package-specific routines or grid search, and model performance was evaluated using R^2 and RMSE on the test sets.

$K_{SW,X}$ predictions were then generated for the new conditions based on field-measured water quality data and predictions from the best-fit model were used to estimate $c_{W,X}$ following Eq. (1). Model details, preprocessing, validation, and model performance parameters (R^2 and RMSE) are provided in *S5A*.

2.8. Comparison between sampling techniques

Agreement between sampling techniques was assessed using a Bland-Altman analysis on log-transformed concentrations obtained from the composite samples, APS and DGT samplers, and visualised through biplots. Data from all three sampling campaigns were combined to evaluate overall comparability of the method across different environmental conditions. Log_{10} transformation was applied to reduce skewness and meet assumptions of the 1:1 correlation.

In addition to the pooled analysis, campaign-specific correlations were also examined to evaluate the consistency of the relationships between the sampling techniques across different sites and sampling periods. Statistical analysis and plotting were performed using GraphPad Prism 10.5.0 (GraphPad Software, USA), and detailed results are provided in *S6*.

3. Results

3.1. *Target compound detection*

Majority of the target compounds were consistently detected in influent and effluent wastewater across the three sampling campaigns, although detection frequencies and concentration ranges varied between locations and years. Most compounds were quantified in the influent samples (data not shown), confirming their continuous input into the wastewater system. Although amphetamine was included in the list of target compounds, its concentrations were consistently below the LOQ in all effluent samples (APS and DGT sorbents and composite samples) across the three sampling campaigns, despite being quantified in influent wastewater samples (data not shown). This suggests efficient removal or susceptible biodegradation of amphetamine during wastewater treatment. In contrast, EDDP (the primary metabolite of methadone), was quantified in Aartselaar in 2023, but concentrations dropped below the LOQ in both influent and effluent samples during the 2024 campaign, likely reflecting reduced methadone consumption or changes in local prescription and usage patterns.

3.2. *Uptake kinetics of psychoactive compounds on passive samplers*

The uptake kinetics of seven target compounds were evaluated across two passive samplers (APS and organic DGT), two sorbents (HLB and MCX), two sampling sites (Aartselaar, Belgium and Ljubljana, Slovenia), and two sampling years for the Aartselaar WWTP (2023 and 2024).

Compounds exhibited curvilinear uptake patterns on the APS and were thus modelled with the exponential equation, whereas linear profiles, mostly observed for the DGT samplers, were fitted using the linear model. As an example, uptake curves for O-desmethylvenlafaxine (ODV) across the sampling campaigns are shown in Fig. 1. Missing data points, e.g., DGT, HLB* and DGT, HLB during the 12-day deployment in the Aartselaar 2023 campaign, were due to the loss of the sorbent material or the entire sampler units during the field deployment, likely caused by strong water currents. Accumulation curves for the other target compounds are displayed in Fig. S7 in the Supplementary Information. Accumulation curves for BZE (2023) were not constructed for DGT samples (<LOQ), while EDDP (2024) was <LOQ in all samples, precluding curve generation.

For the APS system, eventual equilibrium concentrations ($c_{S,\infty}$, nmol L^{-1} as $c_{w,X} \times K_{SW,X}$) and uptake rate constants (k_x) were estimated using Eq. (1) with $c_{S,X}$ (nmol L^{-1}) and deployment time (h) as input data and are summarised in Table 1. Across the sampling campaigns, ODV and tramadol (TRA) showed the highest $c_{S,\infty}$ values, reaching up to 8342 nmol L^{-1} (ODV with MCX, Aartselaar, 2023) and 9764 nmol L^{-1} (TRA with MCX, Aartselaar, 2023). The highest k_x values for HLB and MCX were noted for benzoylecgonine (BZE), particularly in the 2024 sampling, (2.37 and 3.09 × 10^{-2} h^{-1}, respectively).

A unique temporal trend was observed for BZE, both the uptake rate and $c_{S,\infty}$ increased significantly from 2023 to 2024 in Aartselaar across both sorbents. This likely reflects elevated influent and effluent BZE loads during the 2024 sampling period, potentially associated with temporal variations in cocaine consumption within the catchment. In contrast, other compounds generally exhibited significantly lower equilibrium concentrations while uptake rates were slightly lowered. These observed trends are further supported by the aqueous concentrations measured in the composite samples. Moreover, comparable uptake rates were observed for morphine (MOR) across sampling sites and hydroxybupropion (HBP) across sampling years, suggesting stable compound behaviour and consistent sampler performance under the studied conditions.

Sorbent-specific comparisons revealed that MCX enabled faster uptake than HLB for the same compound but lower sorbing capacity as evident from the lower equilibrium concentrations, a general trend that was also observed under laboratory conditions (Anies et al., 2025). This trend was particularly more pronounced in Ljubljana, where MCX exhibited higher k_x for BZE, EDDP, MOR, and ODV compared to HLB. Between sites, Ljubljana had significantly higher MCX uptake rates than Aartselaar for the same compound, e.g., ODV 0.43-0.51 × 10^{-2} h^{-1} for Aartselaar and 1.39 × 10^{-2} h^{-1} for Ljubljana. Conversely, HLB in Ljubljana failed to reach the curvilinear regime for HBP and TRA even after 14 days of sampling. Apparent sampling rates for HBP and TRA estimated using Eq. (2) were 0.29 ± 0.01 and 12.9 ± 1.0 nmol L^{-1} h^{-1}, respectively. These differences may reflect site-specific water characteristics. Specifically, the lower total organic carbon (TOC) levels in Ljubljana (Table S3B) suggest reduced interactions between cationic analytes and organic matter, resulting in less competitive sorption and higher freely dissolved fractions thereby enhancing MCX uptake rates and influencing diffusion toward HLB.

Uptake of most compounds by the DGT samplers followed a predominantly linear trend over the deployment periods. Therefore, the first-order uptake rate constant (k_x) could not be determined. DGT-HLB* (commercial) contains a receiving phase with an agarose gel matrix, while DGT-HLB and DGT-MCX have the same receiving phases as the

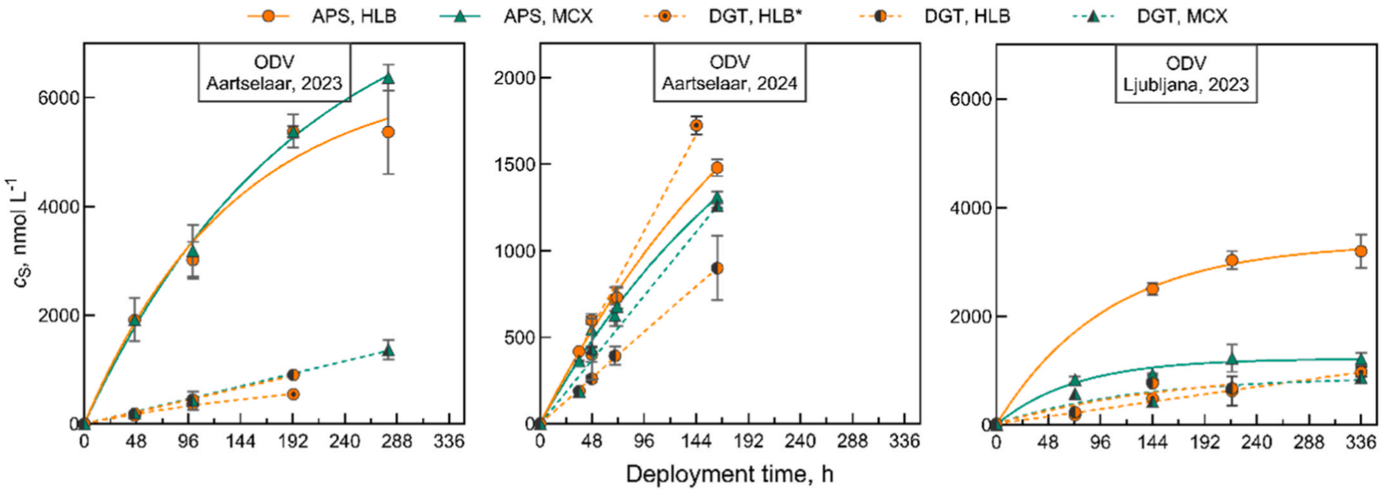

Fig. 1. Accumulated concentrations (c_S, nmol L^{-1}) of O-desmethylvenlafaxine (ODV) on (active) passive samplers with HLB- and MCX-based sorbents across sampling campaigns in Aartselaar, Belgium and Ljubljana, Slovenia. DGT, HLB* is purchased DGT while DGT, HLB and DGT, MCX are lab-assembled with the same sorbent material used in the APS. Error bars represent SD (APS: n = 2; DGT: n = 1 to 3, depending on sorbent recovery).

Table 1

Uptake kinetics of the APS device for psychoactive compounds using HLB and MCX sorbents across sampling campaigns in Aartselaar, Belgium and Ljubljana, Slovenia.

Sorbent	$c_{S,\infty}$ ± se		k_X ± se		R^2	$c_{S,\infty}$ ± se		k_X ± se		R^2	Site
	nmol L^{-1}		$/10^{-2}$ h^{-1}			nmol L^{-1}		$/10^{-2}$ h^{-1}			Year
	Benzoylecgonine (BZE)					EDDP					
HLB	8.8	±0.6	1.04	±0.18	0.97	249	±44	0.42	±0.12	0.98	*Aartselaar, BE*
MCX	5.5	±0.4	1.32	±0.28	0.95	170	±30	0.63	±0.22	0.94	*2023*
HLB	111	±3	2.37	±0.18	0.99	*< LOQ*					*Aartselaar, BE*
MCX	61	±3	3.09	±0.49	0.97	*< LOQ*					*2024*
HLB	89	±16	0.5	±0.17	0.95	762	±171	0.36	±0.13	0.97	*Ljubljana, SI*
MCX	24	±2	1.31	±0.40	0.99	164	±17	2.04	±1.06	0.81	*2023*
	Hydroxybupropion (HBP)					Morphine (MOR)					
HLB	540	±49	0.49	±0.08	0.99	55	±10	1.13	±0.58	0.75	*Aartselaar, BE*
MCX	567	±133	0.36	±0.13	0.97	60	±5	1.26	±0.28	0.94	*2023*
HLB	400	±97	0.34	±0.10	0.98	43	±3	0.79	±0.08	0.99	*Aartselaar, BE*
MCX	245	±53	0.51	±0.15	0.97	40	±5	0.94	±0.18	0.96	*2024*
HLB	*linear*					125	±16	0.57	±0.15	0.97	*Ljubljana, SI*
MCX	151	±13	1.47	±0.40	0.95	63	±7	0.86	±0.23	0.96	*2023*
	O-desmethylvenlafaxine (ODV)					Tramadol (TRA)					
HLB	6449	±712	0.73	±0.17	0.96	7687	±803	0.67	±0.14	0.97	*Aartselaar, BE*
MCX	8432	±853	0.51	±0.09	0.99	9764	±1427	0.51	±0.13	0.97	*2023*
HLB	3009	±465	0.41	±0.08	0.99	3559	±695	0.35	±0.09	0.99	*Aartselaar, BE*
MCX	2603	±553	0.43	±0.12	0.98	2753	±587	0.41	±0.11	0.98	*2024*
HLB	3353	±168	0.99	±0.17	0.99	*linear*					*Ljubljana, SI*
MCX	1224	±81	1.39	±0.33	0.94	944	±133	1.18	±0.53	0.82	*2023*
	Trazodone (TRZ)										
HLB	351	±32	1.02	±0.24	0.94						*Aartselaar, BE*
MCX	346	±38	1.13	±0.34	0.91						*2023*
HLB	98	±18	0.54	±0.13	0.98						*Aartselaar, BE*
MCX	96	±73	0.46	±0.47	0.77						*2024*
HLB	*not measured*										*Ljubljana, SI*
MCX	*not measured*										*2023*

$c_{S,\infty}$ is the equilibrium concentration of the analyte on the sorbent (nmol L^{-1}), k_X is the accumulation rate constant (h^{-1}), se is the standard error of the estimate, and R^2 is to the goodness of fit to *Eq. (1)*.

APS device. In Aartselaar, calculated apparent sampling rates (R_S, nmol L^{-1} h^{-1}) of DGT-HLB and DGT-MCX were similar for all compounds except for EDDP and trazodone (TRZ). Comparing between sampling sites, R_S values for EDDP on both HLB-based samplers were comparable to each other but significantly lower than those for DGT-MCX. In most cases in Ljubljana, DGT-HLB and DGT-MCX samplers generally exhibited a curvilinear uptake pattern and the estimated k_X and $c_{S,\infty}$ values were lower than those measured with APS for the same compounds. Calculated uptake parameters are summarised in Table S7.

3.3. Repeatability of APS and DGT measurements

Repeatability of measurements was assessed during the 2024 campaign where three APS devices containing two sorbents each of HLB and MCX were deployed for six days together with purchased and lab-assembled DGT samplers. The DGT replicates were limited as some receiving phases were lost during the deployment. Consequently, the statistical confidence in these comparisons is limited, and the observed differences between APS and DGT should be interpreted with caution.

Across all compounds, APS and DGT showed comparable measurement consistency for MCX sorbents, while APS-HLB measurements exhibited slightly lower relative standard deviations (%RSD). The %RSD of APS measurements ranged from 1.8% to 6.3% for HLB (n = 6) and 4.4% to 13% for MCX (n = 6), while DGT measurements for some compounds exceeded 10% RSD (Table 2). Interestingly, highest RSDs were observed for more lipophilic compounds, EDDP and TRZ, likely due to diffusion limitations and compound-specific variability in interfacial and sorbent-phase mass-transfer processes at the sorbent-water interface. In contrast, strongly polar compounds such as BZE and MOR, exhibited the highest %RSD with the purchased DGT (DGT-HLB*), a pattern not observed with APS or lab-assembled DGT. This discrepancy is likely due to differences in diffusive gel and membrane composition, HLB embedded in an agarose matrix with a PTFE membrane (for purchased DGT-HLB*) versus a proprietary polymer matrix and PES membrane (for lab-assembled DGTs), which can influence diffusion and partitioning.

Table 2

Repeatability of APS and DGT measurements expressed as %RSD during a six-day deployment.

	Repeatability (%RSD)				
	APS-HLB	APS-MCX	DGT-HLB*	DGT-HLB	DGT-MCX
	(n = 6)	(n = 6)	(n = 3)	(n = 2)	(n = 3)
BZE	1.8	5.6	20	1.8	8.7
EDDP	2.2	13	3.7	11	16
HBP	4.1	4.5	2.7	11	2.7
MOR	2.8	6.8	14	6.1	5.4
ODV	2.5	4.4	3.1	5.4	4.3
TRA	3.1	4.9	3.1	6.3	4.1
TRZ	6.3	13	3.1	35	17

3.4. Conditional K_{SW} prediction by machine-learning

Predictions of sorbent-to-water partition coefficients (K_{SW}) of the seven target compounds across three modelling techniques showed good agreement with measured values (n = 24) (Fig. 2). Among the tested models, machine-learning by XGBoost consistently achieved the highest accuracy having R^2 of 0.84 - 0.99 and RMSE of 0.03 - 0.12 (Table S5A). Random Forest performed moderately better than Bayesian regression

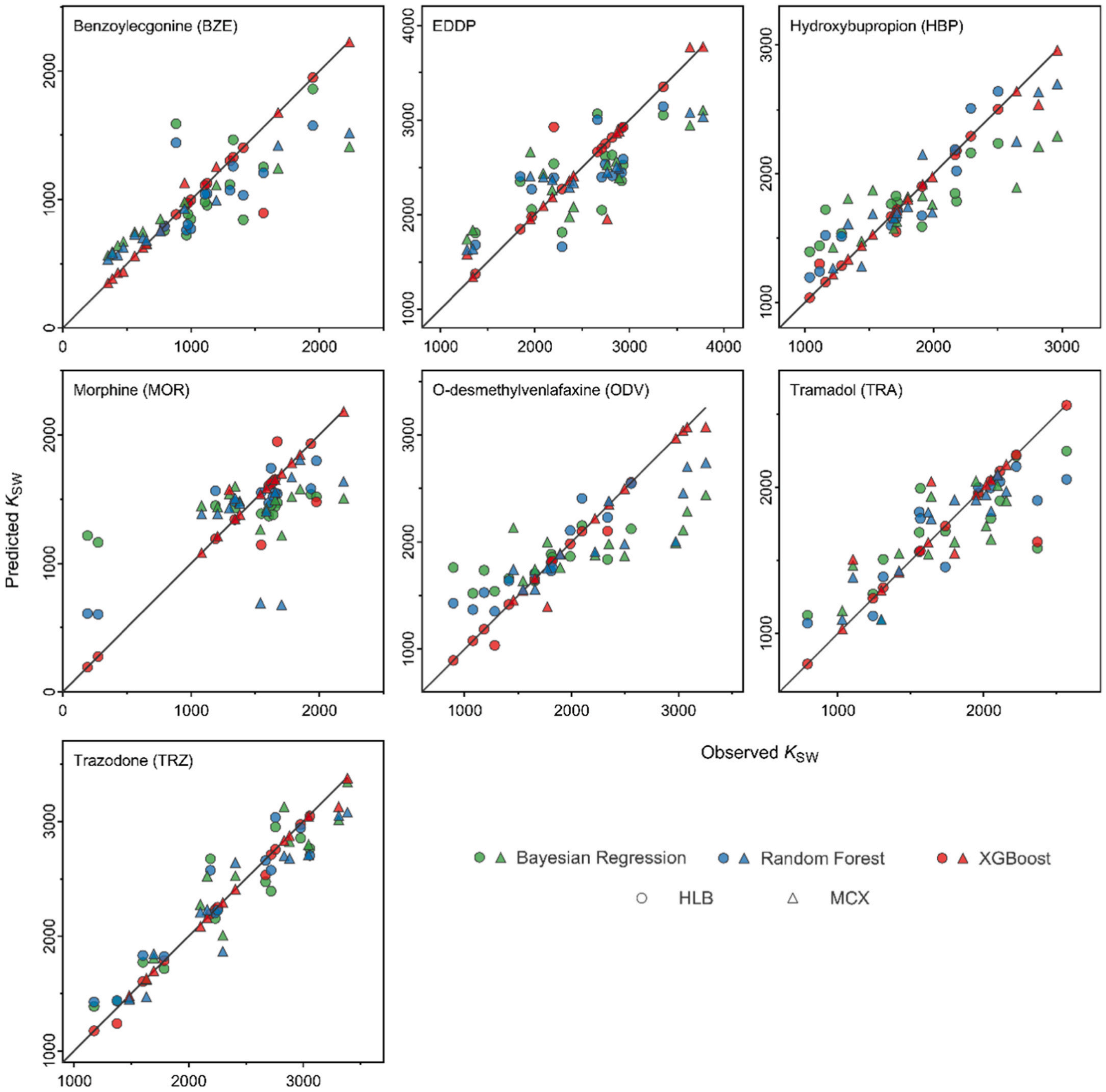

Fig. 2. Predicted vs. observed sorbent-to-water partition coefficients (K_{SW}) of psychoactive compounds on HLB and MCX sorbents using Bayesian regression and machine-learning models (Random Forest and XGBoost).

but both models tended to underestimate higher K_{SW} values and overestimate lower values. Model accuracy varied by compound and sorbent. TRZ had the best fit across the three models ($R^2 > 0.89$) and predictions for MCX tended to be more robust than for HLB.

The superior performance of XGBoost can be attributed to its gradient boosting framework, which creates trees sequentially to minimize residual error and capture complex non-linear interactions among the environmental variables (Chen and Guestrin, 2016). Random Forest relies on averaging independently grown trees, which primarily reduces variance but may retain residual bias. In contrast, Bayesian regression, being a parametric approach, is less flexible in representing non-linear uptake behaviour (Jin et al., 2020; Makalic and Schmidt, 2016). The combination of boosting and regularisation in XGBoost allowed for improved bias-variance trade-off, resulting in more robust and accurate predictions of K_{SW} across compound-sorbent systems. XGBoost produced identical K_{SW} predictions for environmental conditions that were highly similar (e.g., in Ljubljana, water conditions during two sampling periods were pH = 7.86, conductivity = 1016 μS/cm, temperature = 23.0 °C and pH = 7.77, conductivity = 1052 μS/cm, temperature = 22.7 °C) (Table S5B), indicating that the model is robust to minute variations in predictor values.

Despite their predictive strengths, these models are subject to some limitations. Firstly, predictions are constrained by the experimental domain of the dataset and may not extrapolate reliably to environmental conditions beyond those tested, e.g., experimental data were at lower temperatures, 10-15 °C (Anies et al., 2025), whereas field conditions

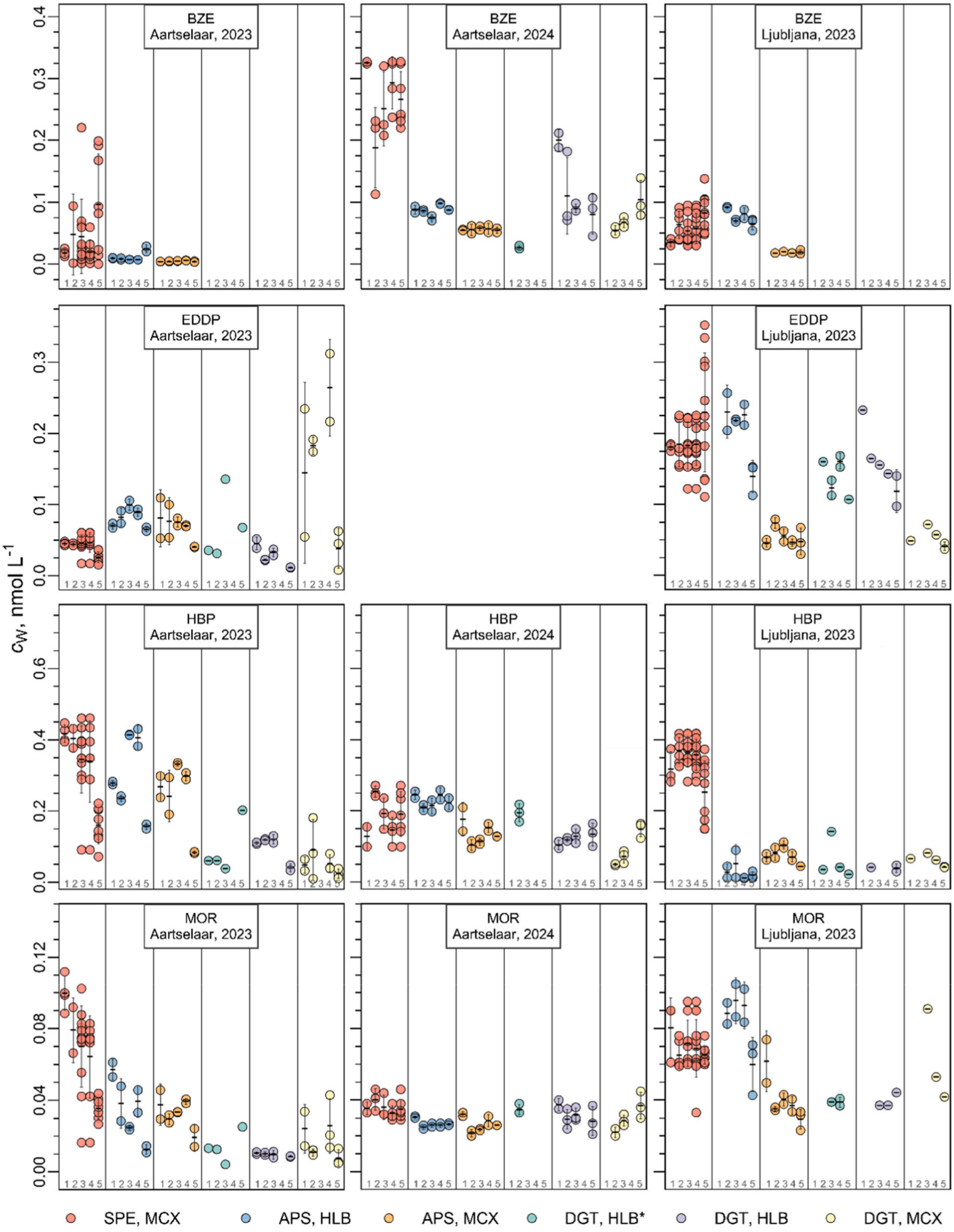

Fig. 3. Aqueous concentrations (c_W, nmol L^{-1}) of psychoactive compounds in effluent wastewater obtained by SPE of composite samples (SPE, MCX), APS (with HLB and MCX sorbents), and DGT (HLB* is purchased DGT, HLB and MCX are lab-assembled DGT) across five deployment periods (sub-columns). In the textbox are abbreviations for psychoactive compounds, locations (Aartselaar, Belgium and Ljubljana, Slovenia), and sampling years (2023 and 2024)

Fig. 3. **(cont.)** Aqueous concentrations (c_W, nmol L^{-1}) of psychoactive compounds in effluent wastewater obtained by SPE of composite samples (SPE, MCX), APS (with HLB and MCX sorbents), and DGT (HLB* is purchased DGT, HLB and MCX are lab-assembled DGT) across five deployment periods (sub-columns). In the textbox are abbreviations for psychoactive compounds, locations (Aartselaar, Belgium and Ljubljana, Slovenia), and sampling years (2023 and 2024).

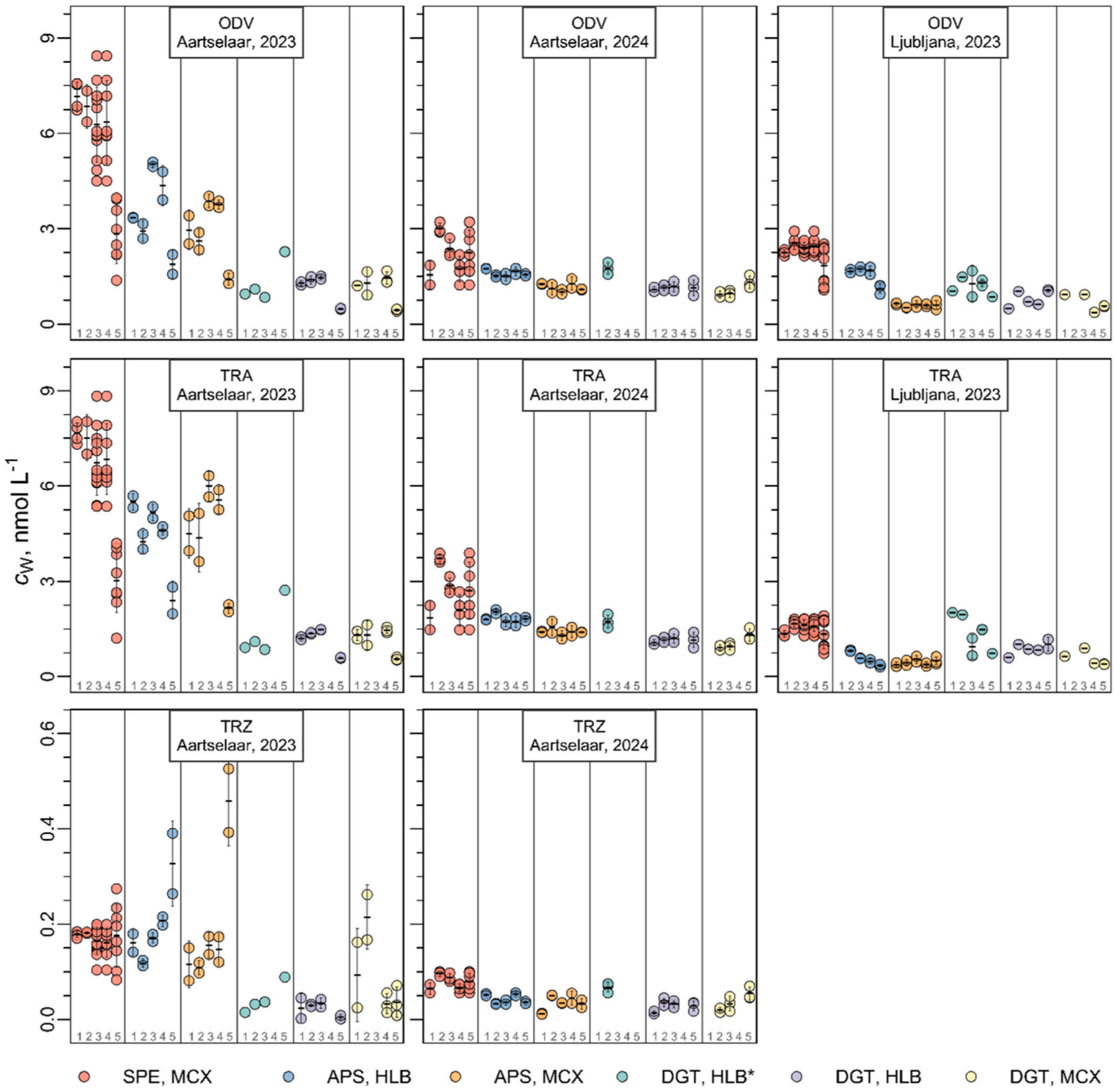

Fig. 3. (*continued*).

were at 16-23 °C. Secondly, machine-learning models depend heavily on the size of the training data, which in this study were limited to a few combinations. Finally, the models inevitably approximate the inherent variability associated with the compound/sorbent properties at different conditions through statistics; thus, information on the mechanistic processes is not available.

3.5. Occurrence of psychoactive compounds in effluent wastewater

Aqueous concentrations (c_W, nmol L^{-1}) were calculated according to the uptake profile of the samplers and using conditional K_{SW} values obtained by XGBoost prediction for those that followed the curvilinear uptake. Concentrations varied depending on the compound, sampling method, and campaign, reflecting differences in use patterns, wastewater treatment conditions, and environmental factors. Concentration patterns and c_W values of the corresponding daily composite samples across the sampling periods are presented in Fig. 3.

3.5.1. Trends across sampling campaigns and locations

Aqueous concentrations of all compounds except for BZE experienced a downward shift in Aartselaar WWTP from 2023 to 2024. This trend was consistent between APS and DGT samplers and mirrored patterns observed in composite samples, suggesting seasonal and/or local usage variations as well as potential influences of wastewater treatment processes. In the same sampling year, Ljubljana wastewater contained higher levels of EDDP, lower levels of ODV and TRA, and similar concentrations of HBP and MOR compared to Aartselaar, which may reflect the larger catchment population and distinct wastewater composition in Ljubljana.

As regular ambient flow rate measurements were not available for both sites, concentration-based comparisons were used as proxies for relative temporal trends. These trends should therefore be interpreted with caution, as flow variability (e.g., rainfall-induced dilution) may influence apparent concentration changes.

3.5.2. Comparison between samplers and sorbents

Across all sampling campaigns, APS and DGT samplers captured generally consistent trends for the seven target psychoactive compounds. In most cases, concentrations obtained by APS are higher than those of DGT, with the highest discrepancies observed in the Aartselaar 2023 sampling, e.g., 2.4-5.5 and 0.6-2.7 nmol L^{-1} for TRA using APS and DGT with HLB sorbents, respectively. For BZE, aqueous concentrations by DGT were not estimated during both 2023 campaigns, as the concentrations in the sorbents were below LOQ.

Considering analytical and sampling uncertainties, differences between HLB and MCX were minor and observed only for selected compounds. The highest sorbent difference was observed for BZE and EDDP during the Ljubljana campaign. EDDP levels ranged from 0.10 to 0.23 nmol L^{-1} using HLB sorbent on both APS and DGT and 0.037 to 0.074 nmol L^{-1} for MCX. Conversely, estimated HBP concentrations in Ljubljana were slightly higher for MCX than for HLB.

3.5.3. Comparison with composite sampling

When compared to conventional SPE of 24-h composite wastewater samples, APS- and DGT-derived concentrations were generally comparable, although composite samples showed higher concentrations for certain compounds during specific deployment periods. During the Aartselaar 2023 sampling, TRA and ODV had the highest concentrations in the water (up to 9 nmol L^{-1}), while on corresponding sampling periods, levels were 30-50% lower for APS and up to 6 × lower for DGT. During the 2024 sampling campaign at the same WWTP, concentrations measured by both passive samplers were generally within the range of concentrations in the composite samples except for BZE. In Ljubljana, a major disparity was observed between composite samples and passive samples for HBP.

4. Discussion

4.1. Active-passive sampling (APS) versus passive sampling

To demonstrate the applicability of APS in wastewater analysis, its performance was compared to that of DGT, a well-established passive sampling approach. While both methods rely on sorbent-based uptake of dissolved contaminants, they differ fundamentally in their sampling mechanisms. DGT sampling in the field is subjected to fluctuating and often uncontrolled hydrodynamic flows, which can influence uptake rates and introduce variability between sites. In contrast, APS is an automated upgrade of passive samplers in which a constant and well-defined flow across the sorbent phase during the sampling is maintained.

The controlled hydrodynamic configuration of the APS is intended to minimize the influence of ambient flow variability. In the present study, APS demonstrated comparable reproducibility to DGT for MCX sorbent and slightly lower variability for HLB sorbent. These findings suggest that APS provides consistent contaminant uptake under the tested conditions, supporting its suitability for passive sampling applications. Nevertheless, the use of APS requires additional logistical considerations, including device maintenance and operational complexity, which may limit its deployment compared to the simpler and more established DGT technique. Moreover, prolonged deployments (>14 days) can result in blockage of the external mesh filter of the device, affecting the water flow to the sorbents, and poor transmission signals at remote sites or heavily-walled effluent catch basins may interrupt the logging of device measurements such as flow rate, water temperature, and air humidity.

The extent to which APS and DGT provide comparable c_W estimates was assessed using Bland-Altman analysis, which allowed for a direct evaluation of the agreement between the two methods. While DGT sorbent loss during some deployments resulted in fewer replicates per sorbent type, the pooled Bland-Altman analysis across all compounds remains robust. Shown in Fig. 4 are the biplot comparisons between APS and DGT and in Table S6 are the bias and limits of agreement. For the pooled data, APS generally presented higher uptakes than DGT. APS-HLB measurements showed biases of 1.66 and 1.82, indicating that APS measurements were 66% and 82% higher than the purchased and lab-assembled DGT-HLB, respectively. Using the MCX sorbent, APS measurements were 35% higher than those of DGT. However, a relatively high SD of the bias further suggests that individual measurements can differ substantially between methods and sorbents.

Campaign-specific correlations revealed that APS measurements were 2 to 3 times higher than DGT measurements during the 2023 campaign in Aartselaar. At the same site in 2024, the differences were markedly reduced, with APS measurements only 11 to 23% higher than DGT. This reduction may be related to the shorter deployment periods in 2024, which could have limited the influence of fluctuating flow currents on DGT performance. However, variations in effluent composition and the known sensitivity of DGT to hydrodynamics under low flow conditions may also have contributed. Moreover, APS measurements in

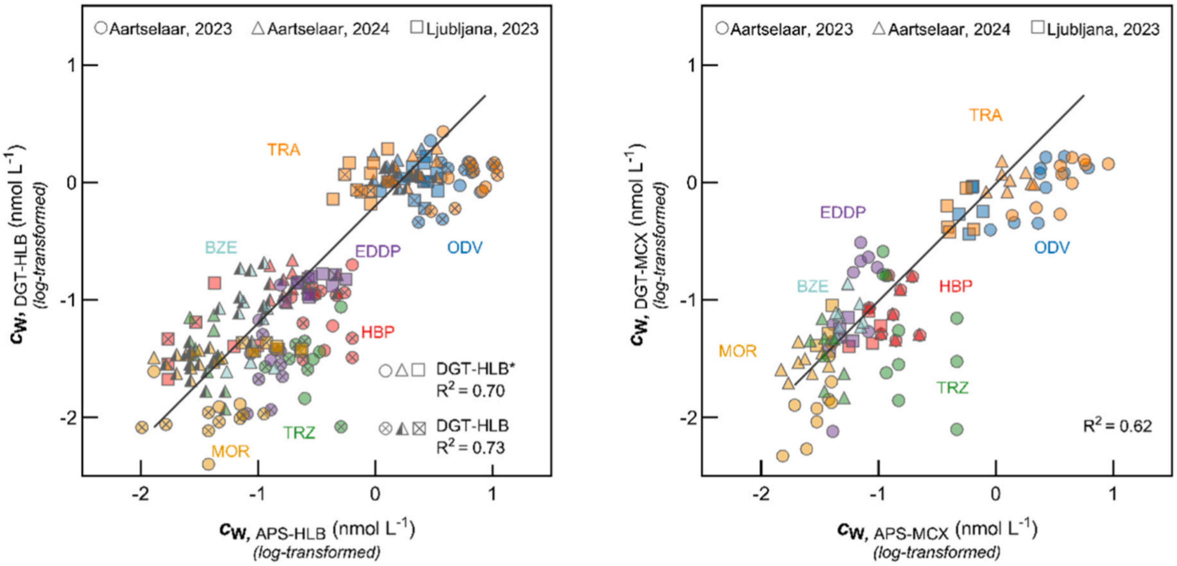

Fig. 4. Comparison of aqueous concentrations (c_W, nmol L^{-1}, log-transformed) of psychoactive compounds in effluent wastewater obtained by APS (with HLB and MCX sorbents) and DGT (HLB* is purchased DGT, HLB and MCX are lab-assembled DGT) across sampling locations (Aartselaar, Belgium and Ljubljana, Slovenia) and sampling years (2023 and 2024).

Ljubljana differed by only about 6 to 11% compared to DGT. Measured water quality parameters indicated slightly higher pH and more stable conductivity in Ljubljana, while Aartselaar wastewater exhibited higher TOC and greater variability in conductivity. These differences in organic matter content and ionic strength may partially explain site-specific variations in passive sampler uptakes.

Organic DGT (o-DGT) has been successfully applied to pharmaceuticals and other organic pollutants, with several studies emphasising the importance of deployment conditions for accurate uptake (Challis et al., 2016; Fialová et al., 2024; Liu et al., 2021). A key factor is the diffusive boundary layer (DBL), which is strongly influenced by water flow. It was showed that at low to moderate water velocities (<2 cm s^{-1}) the DBL can significantly affect the solute transport (up to 50% reduction of the true concentration), while at higher flows (>2 cm s^{-1}) the DBL formation becomes negligible for diffusive gels of ≥ 0.7 mm thickness (Gimpel et al., 2001; Uher et al., 2013). As water flow rates at the effluent catch basins were not recorded and hydraulic conditions were variable, the DBL thickness could not be reliably estimated. Hence, in the standard DGT interpretation, the contribution of the DBL is often considered negligible under typical deployment conditions (Zhang and Davison, 1995), though at low or variable flow this assumption may not hold.

4.2. Active-passive sampling versus composite sampling

While composite sampling followed by SPE remains the routine method in wastewater monitoring, it typically captures total concentrations that include both dissolved and particle associated fractions. In contrast, APS, like other passive samplers, can selectively accumulate the freely dissolved/bioavailable fractions which are responsible for uptake by organisms, degradation, and transport in aquatic systems (Amato et al., 2021; Fedorova et al., 2014; Shakallis et al., 2022).

Suspended particulate matter (SPM) may influence the transport and sorption of certain psychoactive compounds to passive samplers by affecting particle-sorbent interactions. SPM was not characterized during the current field campaigns, so its effect cannot be directly verified. Previous work (Anies et al., 2025) suggests that SPM can alter compound partitioning under controlled conditions. Detailed modelling results using these data for the environmental conditions encountered in the field sampling are provided in the Supplementary Information (*S5B*). In the present study, aqueous concentrations were calculated using the *no-SPM* predictions, and SPM effects are discussed as a potential contributing factor to observed differences between APS and composite sampling.

According to the Bland-Altman analysis, CS/SPE measurements were generally higher than APS measurements with differences of 55% and 121% for HLB and MCX sorbents, respectively. This trend is consistent across the three sampling campaigns (Fig. 5, Table S6). The higher bias observed for MCX is likely linked to differences in sample treatment. Composite samples were filtered through GF filters (Slovenian samples) and acidified (Belgian and Slovenian samples) before SPE. Acidified samples were typically loaded immediately onto the cartridges, and the duration of the acidification step was governed by routine sampling handling rather than by a set timing. The effective contact time between sample and sorbent is operationally defined by the sample volume and vacuum-assisted flow through the cartridge, rather than by a controlled equilibration period, and is generally not standardized in routine SPE protocols. Therefore, it was not possible to determine the extent of dissociation of the particle-bound psychoactive compounds during this pre-treatment step. In contrast, APS deployments in the field do not modify the pH of the sampled medium. This further suggests that MCX in situ may be more sensitive to water quality parameters and possible electrostatic interactions with other cationic contaminants in the wastewater. It is possible that stronger cations may have saturated the cation exchange sites of MCX, adding complexity to the sorption of the target psychoactive compounds. However, this aspect was not further investigated in this study. Field measurements of water quality showed that the pH of the sampled wastewater was in the range of 7.0-8.0, conductivity spanned 300-200 μS/cm, total organic carbon (TOC) was 13-47 mg/L, and temperature was 16-23 °C (Table S3B). The variable and uncontrolled environmental conditions encountered during the field deployments highlight the inherent complexity of interpreting APS and other passive sampling results, where observed differences may reflect both actual chemical concentrations and environmental influences on sampler uptake.

5. Conclusion

This study evaluates the applicability of an active-passive sampling (APS) approach for monitoring the occurrence of psychoactive compounds in effluent wastewater, integrating field deployments with predictive modelling of sorbent-to-water partition coefficients (K_{SW}). Moreover, APS measurements reliably captured aqueous concentrations

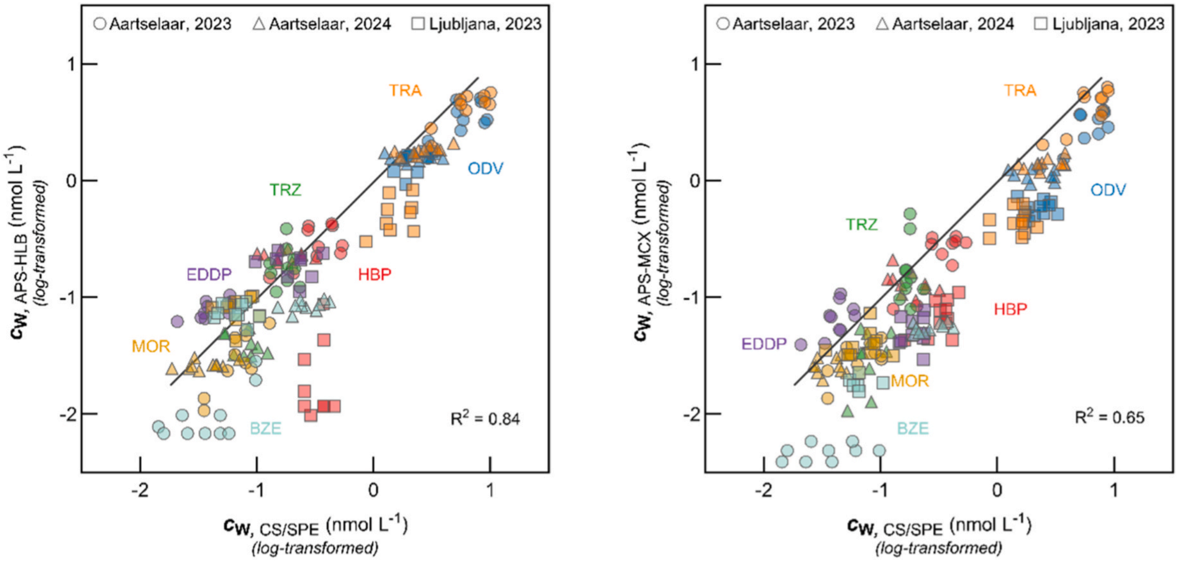

Fig. 5. Comparison of aqueous concentrations (c_W, nmol L^{-1}, log-transformed) of psychoactive compounds in effluent wastewater obtained by composite sampling-SPE (with MCX sorbent) and APS (with HLB and MCX sorbents) across sampling locations (Aartselaar, Belgium and Ljubljana, Slovenia) and sampling years (2023 and 2024).

and showed good agreement with DGT measurements, although differences were influenced by the type of sorbent and environmental conditions. Comparisons with composite sampling-SPE highlighted the complementary nature of these approaches, with APS providing information on bioavailable fractions and possible influence of particle associations. Predictive modelling using XGBoost provided a realistic estimation of K_{SW} under varying conditions, supporting the interpretation of samplers operating at near-equilibrium uptake. Overall, APS offers a robust alternative monitoring tool towards understanding contaminant fate in aquatic systems.

CRediT authorship contribution statement

Allen Jun Anies: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Maria Laimou-Geraniou:** Writing – review & editing, Methodology, Investigation, Formal analysis. **Maarten Quireyns:** Writing – review & editing, Methodology, Investigation, Formal analysis. **Tim Boogaerts:** Writing – review & editing, Validation, Supervision. **Cara Byns:** Writing – review & editing, Supervision. **Taja Verovšek:** Validation, Supervision. **David Heath:** Writing – review & editing, Validation, Supervision, Investigation. **Ester Heath:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Funding acquisition. **Alexander L.N. van Nuijs:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Funding acquisition. **Adrian Covaci:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Funding acquisition. **Ronny Blust:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Funding acquisition, Conceptualization. **Raewyn M. Town:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Funding acquisition, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

We acknowledge the financial support of the Research Foundation-Flanders (FWO) (G060920N, 1148622N, 1225924N), and the Slovenian Research and Innovation Agency (P1-0143, N1-0047, L7-4422). We extend our gratitude to the technical staff of the wastewater treatment plants in Aartselaar, Belgium and Ljubljana, Slovenia for their support during the field campaigns, with special thanks to Birte Raes and Vesna Mislej for their exceptional assistance and expertise.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envpol.2026.127930.

Data availability

Data will be made available on request.

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