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Research article

Soil organic matter decomposition as a key driver of pharmaceutical retention

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ABSTRACT

Human activities release Pharmaceutically Active Compounds (PhACs) onto arable land, where they can accumulate and disrupt the ecological balance. The soil's microbial community continuously alters the composition of organic matter, as it serves as their primary nutrient source. The quality and quantity of organic matter may vary even within a single vegetation period. Observing the extent of transformation in the different phases is essential, as organic matter is primarily responsible for the soil's ability to retain micropollutants. An incubated sorption experiment was conducted simulating a vegetation period using Mollisol, to examine this question. Enzyme activity results indicate that the microbial community transforms soil organic matter, reducing its quantity and thus its ability to retain PhACs. At the beginning of the incubation period, among the physicochemical properties of PhACs, the H-donor/acceptor counts and the size of their van der Waals surface area were the determining factors in the sorption processes. At the end of the incubation period, owing to the reduction in organic matter and the transformation of functional groups, the adsorbed PhACs decreased significantly, while desorption increased because the electrostatic interaction began to dominate the sorption processes. Consequently, the mobility rate of the PhACs with hydrophobic properties may increase in the arable land by the end of the vegetation period. The primary properties of PhACs identified should be considered when assessing soil persistence. It's vital to account for the temporal evolution of soil conditions and avoid relying on a single observation, as this only partially represents the soil's actual state.

1. Introduction

Globally, Mollisols cover 8,308,734.5 km^2 and are located predominantly in the northern hemisphere (Fig. 1) (Yakutina et al., 2015). These locations are used primarily as arable land, and account for around 29.2 % of total global arable soils, a proportion which is rapidly rising due to increasing agricultural demand driven by population growth (Schneider et al., 2011; Shang et al., 2012). To meet this escalating necessity, there is a growing reliance on the use of treated wastewater for irrigation, while sewage sludge and livestock manure are both utilized for soil nutrient replenishment (Morugán-Coronado et al., 2011; Szabó et al., 2024). However, these recycled resources are often polluted with highly persistent pharmaceuticals and their metabolites, which accumulate during wastewater treatment processes (Martínez-Alcalá et al., 2018a; Westhof et al., 2016; Ojobe et al., 2021). These metabolites, which can be as dangerous as the parent compounds, contribute to soil and water pollution. However, their bioavailability, co-metabolic transformation and mechanisms of action in the subsurface

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environment (e.g. rhizosphere) remain poorly understood, especially regarding their effects in combination with their parent compounds on different ecosystems (e.g. agro-ecosystems) (Mejías et al., 2021; Martínez-Alcalá et al., 2018b; Zhang et al., 2021; Jelic et al., 2011; Szabó et al., 2020; Nguyen et al., 2021, 2023; Filep et al., 2021). Nevertheless, these compounds, with mutagenic and carcinogenic properties, are recognized as harmful contaminants in the soil environment (Ramanayaka et al., 2023). The accumulation of Pharmaceutically Active Compounds (PhACs) in soils can lead to species extinction, disrupt food chains, and cause bioaccumulation in crops, which poses significant ecological and health risks (Carter et al., 2014). These impacts also threaten agriculture by reducing crop quality and yield, leading to economic losses and potential market restrictions (Cuthbert et al., 2011; Paudel et al., 2016; Qiang et al., 2016; Yan et al., 2017).

Many environmental chemistry studies examine soil organic matter (SOM) only as a discrete sample, taken at a specific moment, a "snapshot", which cannot capture the temporal changes in SOM dynamics or their influence on the sorption of PhACs during a vegetation period (Graouer-Bacart et al., 2016; Fenet et al., 2012; Mrozik and Stefańska, 2014; Kodešová et al., 2015; Wu et al., 2022). Moreover, the diversity of SOM supply is limited, as the particulate organic matter (POM) deposited in soil is produced by a restricted range of plant species (e.g., vascular plants). In addition, agricultural practices, such as harvesting, often involve the removal of most POM sources; namely, crops that further limit the input of fresh organic matter (OM) into the soil. The constrained availability of POM, and SOM degradation by soil microbial communities (SMC) simultaneously leads to a steady decline and continuous physicochemical transformation of existing SOM (Lal, 2020; Mrabet et al., 2001). These bacterial and fungal communities are heterotrophs, i.e., they derive their energy and carbon source from SOM; thereby, affecting various transformations in SOM, e.g. changes in the ratio of the aliphatic-aromatic-phenolic functional groups (Erdel et al., 2023; Chen et al., 2018). Owing to these phenomena, the composition and amount of SOM in agricultural soils change both spatially and temporally. As a result, the effect of the constantly changeable nature of SOM on PhACs retention remains under-researched.

In soil solution systems, the primary and secondary intermolecular interactions between organic contaminants and colloidal particles are governed by the quality of the adsorbent (the soil) and the physicochemical properties of the adsorbate (the PhACs). These parameters simultaneously shape the sorption dynamics of PhACs within the soil matrix (Nguyen et al., 2021, 2023; Vancsik et al., 2024). From the adsorbent's perspective in soils with an organic fraction exceeding 0.1 %, such as Mollisols, SOM surface chemistry—including its polarity, aromaticity, and aliphaticity—along with its quantity, plays a decisive role in regulating retention due to specific PhACs-SOM associations (Qin et al., 2017; Estevez et al., 2014). These properties facilitate complex interactions with PhACs, enhancing their sorption processes. In contrast, soils with lower SOM concentrations exhibit reduced retention capacity due to the lack of available adsorption sites (Alhalabi et al., 2024; Hickey et al., 2024).

SOM represents a continuum of organic compounds at varying stages of decomposition, from intact plant material (the POM) to highly oxidized forms like carboxylic acids (Lehmann and Kleber, 2015; Trumbore, 1997). Along this continuum, biopolymers with distinct aliphatic or aromatic structures uniquely influence the sorption processes of PhACs. As SOM decomposition follows a thermodynamic gradient, energy-rich compounds degrade into smaller, energy-depleted molecules. Each phase of this decomposition process, which is driven by shifts in the ratio of aliphatic to aromatic compounds, has an impact on the sorption behaviour of organic micropollutants (Ramanayaka et al., 2023; Lehmann and Kleber, 2015; Filep et al., 2024). On the adsorbate side (PhACs), their physicochemical properties determine the adsorption-desorption processes, e.g., acid dissociation constant (pKa), pH-dependent lipophilicity ($\log_D$), van der Waals surface area (vdWSA), the number of aliphatic/aromatic bonds (nAlb/nArb) and H-bond donors/acceptors (nHBD, nHBA) (Szabó et al., 2020, 2024; Zhang et al., 2021; Filep et al., 2021; Ramanayaka et al., 2023; Vancsik et al., 2024; Franklin et al., 2022). Hereafter, we denote the hydrogen-bond donor/acceptor ratio as nHBda (nHBda = nHBD/nHBA). However, in contrast to the adsorbent (soil), the physicochemical properties are PhACs-specific, retaining consistent characteristics when repeatedly released into the subsurface environment. The most common intermolecular reactions in soil-colloid systems are usually hydrophobic interactions (H-bonding, van der Waals forces, surface complex formations and electrostatic interactions, cation exchange and cation bridges) (Filep et al., 2021; Franklin et al., 2022). PhACs can also interact with each other, i.e., they can be competitive partners, antagonistically decreasing or synergistically increasing each other's sorption activity (Szabó et al., 2024; Kodešová et al., 2023). With the continuous

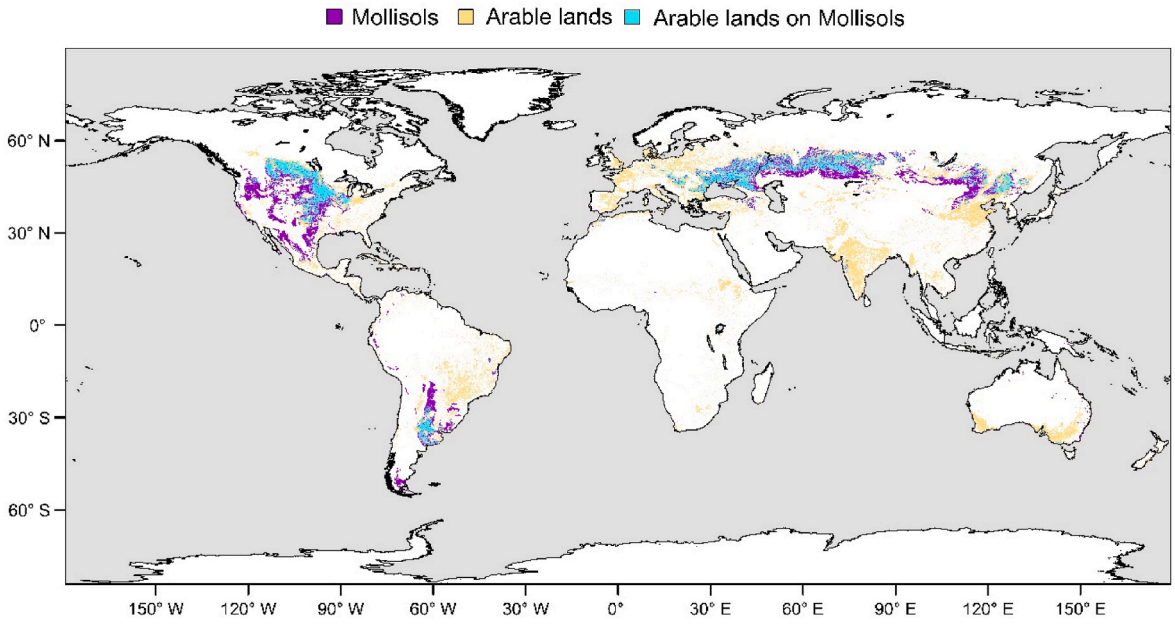


Fig. 1. Global distribution of Mollisols and arable lands (Based on the FAO database (Food and Agriculture Organization of the United Nations (FAO))**).**

transformation of SOM, the frequency and distribution of these complex interactions may change and affect the terrestrial transport and the bioavailability of PhACs in the rhizosphere (Zhang et al., 2021; Kodešová et al., 2023). Due to the influence of SOM, a deeper understanding of the sorption of PhACs in arable lands would be needed in order for their bioavailability to be predicted more accurately (Zhang et al., 2021).

In this study, we simulated a vegetation period using a Mollisol and used PhACs with diverse physicochemical properties that cover a wide range of the characteristics typical of PhACs that are accumulating within the rhizosphere, such as (Carbamazepine (CBZ), 17α-ethynylestradiol (EE2), and Diclofenac-sodium (DFC)) and their metabolites (trans-10,11-Dihydro-10,11-dihydroxy Carbamazepine (TCBZ), Estrone (E1), Estriol (E3), 17β-Estradiol (BE2), 17α-Estradiol (LE2), and 5-Hydroxydiclofenac (5HODFC)). We performed separate fixed-bed experiments (15 columns) to determine the main sorption properties of PhACs at the beginning, middle and end of the simulated vegetation period. In parallel, we monitored changes in SOM as characterized by indicator physicochemical parameters (e.g. changes in soil organic carbon (SOC), the ratio of dissolved organic carbon (DOC) to SOC, representing a labile and readily available pool of SOM for microbial activity (Yang et al., 2017; Wang et al., 2022; Li et al., 2018), and the composition of soil aliphatic and aromatic compounds), plus the SMC properties (e.g. acidic phosphatase and dehydrogenase enzyme activity, and the composition of the communities). Chemometric modelling allowed us to visualize how the physicochemical properties of PhACs influence the sorption processes at different stages of SOM decomposition. The comprehensive multivariate approach allowed us to model and interpret the complex interactions between soil, SMC, and adsorption parameters in a robust way, providing new insights into the time-dependent behaviour of PhACs in soil matrices.

With these data, we estimate to what degree parent compounds and their metabolites are retained and released by the ever-changing OM medium. This study provides the first evidence that the temporal degradation of SOM within a single vegetation period can significantly alter the sorption behaviour and mobility of PhACs in soil. By combining long-term incubation with chemometric modelling, we show that both the quantity and quality of SOM change over time, which in turn shifts the dominant physicochemical properties that control PhACs retention. Nevertheless, the primary objective of this study is to investigate how temporal changes in SOM decomposition within a single vegetation period affect the sorption behaviour and mobility of PhACs in soil. The mobility and thus the environmental risk of specific PhACs may increase or decrease depending on the progression of SOM transformation. We can identify the key SOM fractions that influence these shifts, offering new insights into the time-dependent nature of contaminant–soil interactions. These findings not only contribute to a deeper understanding of pollutant behaviour in dynamic soil systems, but may also be used to simulate the temporal mobility of PhACs in agricultural environments, thereby informing the long-term management of soil nutrient replenishment and contaminant risk.

2. Materials and methods

2.1. Selected PhACs

This study focused on three pharmaceuticals (CBZ, EE2, DFC), each possessing distinct physicochemical properties. These differences enable them to establish varied intermolecular interactions with the adsorbent (soil). Furthermore, these compounds encompass the physicochemical characteristics most associated with PhACs found in the environment. Consequently, they serve as representative compounds for estimating the environmental behaviour and fate of PhACs. Further, given the intensive abiotic and biotic degradation processes occurring in soils, we extended our analysis to include the sorption processes of the primary degradation products of these parent compounds, such as TCBZ, E1, E3, BE2, LE2, and 5HODFC. High purity (≥99 %) analytical standards were purchased from Sigma-Aldrich (Sigma-Aldrich, USA).

2.2. Study site and soil sampling

A set of five Mollisol samples was collected using composite sampling methods (ISO 18400-107:2017) from a patch of uncultivated arable land on the Heves Plain in Hungary (47°40′13.0"N 20°21′54.3"E, 47°40′13.4"N 20°21′53.8"E, 47°40′13.6"N 20°21′54.9"E, 47°40′12.8"N 20°21′55.1"E, and 47°40′12.5"N 20°21′54.0"E). Further information about Mollisol and climatic conditions can be found in the Supplementary Materials (Text S1). Composite sampling involved pooling subsamples from these points across the site to minimize the influence of spatial variability and ensure a more accurate representation of the general soil properties of the typical Mollisol. The samples were collected from the rhizosphere (plough layer, 0–20 cm), where soil-root interactions are most active. Because of the specific site has not yet been used for agricultural cultivation due to local accessibility issues, this means they are free from PhACs and other anthropogenic pollutants and serves as an ideal reference for baseline soil characteristics. Preliminary measurements using UHPLC confirmed the absence of nine target PhACs in the soil samples. For this, representative composite samples were extracted with methanol:ultrapure water (80:20 v/v), followed by ultrasonication, centrifugation and filtration. The resulting extracts were analyzed with a Shimadzu Nexera X2 UHPLC with a Kinetex® XB-C18 column (Shimadzu, Japan). None of the compounds were detected above their respective detection limits. Additionally, on each sampling day, PhACs-free water was poured through a blank soil sample to monitor the leaching of targeted PhACs (Text S5).

The Heves Plain, Hungary, was chosen due to its agricultural significance, with 76.4 % of the land on it used for arable farming. This region was selected to ensure that the results are relevant to regional land management and soil conservation efforts, with composite sampling employed to mitigate any potential site-specific biases and achieve standardized, representative data (Ambrózy et al., 2010). The map (Fig. 1) indicating the presence Mollisols and arable land areas was created using the FAO database. The map was created using ArcGIS 10.8 software.

2.3. Experiments

The experiment consisted of three phases (Yakutina et al., 2015): soil chemistry measurements (Schneider et al., 2011); enzyme activity and SMC diversity of soil; and (Shang et al., 2012) adsorption-desorption of PhACs. All experiments were performed simultaneously and stored in an incubator.

2.4. Soil characteristics and measurements

(1) Soil samples were prepared by removing roots and plant debris larger than 2 cm. Soil sieving through a 2 mm Fritsch analytical metal sieve was performed to standardize grain sizes and minimize their influence on sorption processes (ThermoFisher Scientific, USA). For soil chemistry, fifteen soil samples weighing 5 g each were incubated in triplicate in borosilicate glass tubes (Sigma-Aldrich, USA). The incubation period was set at 92 days in a climate chamber (ILW 240 STD, Sigma-Aldrich, USA). During incubation, samples were maintained in darkness with a constant soil water holding capacity and temperature set at 20 °C ± 1 °C. The soil samples were kept at 70 % of their field water-holding capacity throughout the incubation period by adding distilled water every three days (Yang et al., 2021a). The top of the borosilicate glass was linked to the air vent by a three-way valve.

On days 0, 14, 28, 42, 92 various parameters were measured to characterize the soils. The pH of the soil-water suspension was determined using a glass electrode according to the MSZ-08-0206/2 standard (Table S2) (PONSEL Odeon combined electrodes, Sigma-Aldrich, USA).

SOC %, m/m content and nitrogen content (TbN %, m/m) were quantified using a CHNS elemental analyzer (Elementar varioMacro cube, Germany). The carbon-to-nitrogen ratio (C/N) was calculated based on these measurements. An IC analyzer (Shimadzu SSM5000A, Japan) was employed to determine the inorganic carbon (IC %, m/m) content. Physical properties such as clay, silt, and sand percentages were determined using a laser diffraction particle size analyzer (Malvern Mastersizer 3000; refractive index: 1.54, absorption coefficient: 0.1, United Kingdom) (Gresina, 2020). The mineral composition of the soil was analyzed using X-ray powder diffraction (XRD) measurements conducted on a Rigaku Miniflex 600 instrument (Tokyo, Japan). Fourier Transform Infrared (FT-IR) spectroscopy in the DRIFT mode with an RT-DLaTGS detector (Bruker Vertex70, Massachusetts, USA) was employed to characterize the composition of SOM, specifically identifying aliphatic and aromatic components.

2.5. Enzymatic activity and SMC measurements

(2) Soil samples were incubated under controlled conditions, and enzyme activities (dehydrogenase (DHA) and acid phosphatase enzyme (ACP)) were measured using spectrophotometric methods, while microbial communities were analyzed through DNA extraction, PCR amplification, and amplicon sequencing. OTUs were identified based on 16S rRNA gene and fungal ITS region, and data were processed to exclude poor quality sequences. The details of the enzyme activity and SMC measurements can be found in the Supplementary Materials (text S2).

2.6. Adsorption-desorption experiments

(3) Fifteen columns were prepared and incubated for adsorption-desorption experiments. On each sampling day (0, 14, 28, 42, and 92), separate fixed-bed experiments were carried out in triplicate using borosilicate glass columns (ThermoFisher Scientific, USA) with a 10 mm inner diameter (Fig. S3). Preliminary tests determined that 2 g of adsorbent was appropriate due to the high adsorption affinity for PhACs. To prevent washout and edge effects, inert glass wool was placed both above and below the adsorbent (soil). A peristaltic pump was used to manage the flow rate, maintaining it at 2 ml/min downstream (LEA BT100F, Lead Fluid (Baoding) Intelligent Equipment Manufacturing Co., Ltd., China). The concentration of the influent PhACs was consistently 0.1 μg/ml/PhAC in all experiments. According to OECD guidelines, compounds with low aqueous solubility (e.g., CBZ and EE2) were initially dissolved in methanol as co-solvent to prepare stock solutions, which were subsequently diluted with ultrapure water. The concentration of the influent PhACs was consistently 0.1 μg/mL per compound in all experiments. This concentration was selected based on preliminary trials as the optimal level for detecting competitive interactions while remaining within environmentally relevant ranges, particularly for Mollisol soils potentially exposed to treated wastewater, sewage sludge, and surface runoff. The chosen level also complies with OECD recommendations and ensures sufficient analytical sensitivity for UHPLC-quantification without additional sample pre-treatment. Competitive sorption experiments were performed with all nine molecules present simultaneously in the liquid phase. During the fixed-bed experiments, effluent samples were collected in 10 mL fractions for subsequent analysis. The supernatants were filtered using 0.45 μm glass fiber filters (Chromafil® GF/PET-45/25, Sigma-Aldrich, USA). Effluent samples from the column were collected and analyzed at specific intervals using Ultra-High-Performance Liquid Chromatograph (UHPLC, Shimadzu, Nexera X2 LC 30-AD, Japan) with a fluorescence detector (Shimadzu, RF 20 A XS) and a C18 core-shell column (Kinetex®, 2.6 μm XB-C18) (Table S7). The detection limits (LOD) and quantification limits (LOQ) for CBZ, EE2, and DFC were determined as 25.10, 2.27, 6.70 ng/L and 76.10, 6.89, 20.40 μg/L, respectively (Table S7). The performance of the fixed-bed columns was assessed using breakthrough curves, with the breakthrough point occurring at 5 % of the initial concentration (C_0) and full saturation being defined when 95 % of the adsorption sites were occupied by the PhACs (Patel, 2022; Bauer et al., 2025). The column was cleaned by rinsing with 5 ml of ultrapure water, followed by flushing with a 0.01 M $CaCl_2$ solution to fully desorb the reversibly bound PhACs (Szabó et al., 2024; Vancsik et al., 2024).

2.7. Calculation of the sorption parameters

During adsorption measurements, the following parameters were calculated for each PhACs on every sampling day (0, 14, 28, 42, and 92 days): Quantity of the adsorbed PhACs in time (q_{ti}), Break time (T_{break}), Saturation time (T_{sat}), Maximum adsorption capacity at the moment of complete saturation (q_{max}), Total bed adsorption capacity (q_{total}), Adsorption area (A_{area}), Desorption area (D_{area}), Total bed desorption capacity (qd_{total}), Desorption percentage (Pd%) (Tables S3–S5). Calculations of the parameters are detailed in Text S3.

2.8. Statistical analysis

We conducted statistical analyses to examine the relationships among soil parameters, adsorption–desorption parameters, and SMC variables across the sampling days. First, the normality of all variables was tested using both the Shapiro–Wilk and Lilliefors tests ($p < 0.05$) (Mohd Razali and Bee Wah, 2011). Variables meeting the normality criteria were subjected to Repeated Measures MANOVA ($p < 0.05$) to determine whether significant differences occurred across the sampling days (0, 14, 28, 42, and 92). Subsequently, Pearson correlation analysis was performed to investigate the relationships between soil and SMC parameters. We considered correlation coefficients above 0.7 or below −0.7 as indicative of strong statistical associations between variables.

To ensure comparability, the dataset was standardized to a mean of 0 and a variance of 1, following established methodologies (Canteral et al., 2023). Canonical Correlation Analysis (CCA) was then applied to model the time-dependent variation in PhACs sorption dynamics by correlating the adsorption-desorption parameters with the physicochemical properties of the various PhACs. Through CCA, we extracted canonical correlations between the two variable groups (U: adsorption-desorption parameters, (Text S4. Eq. (7)); V: physicochemical properties (Text S4. Eq. (8)), which allowed us to interpret how these sets of variables interacted over time. Within these analyses, we computed two canonical correlations between the U and V variable sets: D1, representing the strongest linear relationship between the canonical variables, and D2, representing the second strongest correlation (Canteral et al., 2023). To interpret the CCA results further geometrically, we applied an orthogonal rotation to the canonical variables, and investigated how the charges (canonical weights) of a set of vectors (variables V and U) in the CCA varied over time (as a function of sampling days).

To gain a deeper understanding of how the physicochemical properties of PhACs influence sorption dynamics over time, the canonical scores obtained from CCA were subjected to Hierarchical Cluster Analysis (HCA). This analysis enabled us to explore the temporal evolution of variable importance, revealing how certain physicochemical properties became more influential as the system evolved.

All statistical analyses, including MANOVA, Pearson correlation, CCA and HCA, were performed using the RStudio (4.4.1) Team (2020), with additional support from Origin 2023Pro, and Seed software (version 2.1.1.). This comprehensive multivariate approach allowed us to model and interpret the complex interactions between soil, SMC, and adsorption parameters in a robust way, providing new insights into the time-dependent behaviour of PhACs in soil matrices.

3. Results

3.1. Temporal changes in SOM content and SMC

We measured the SOM and SMC parameters, during the incubation, at five time points 0, 14, 28, 42, and 92 days. Our research concentrated on the qualitative and quantitative alterations within SOM, including a reduction in SOC, the ratio of DOC to SOC, and a modification in the composition of soil aliphatic (Lehmann and Solomon, 2010), aromatic compounds (Demyan et al., 2012) and phenolic lignin compounds (Veum et al., 2014). SMC dynamics were assessed via DHA and ACP activity assays. Changes in the prokaryotes and the fungal communities, in the enzyme activities, and in soil parameters are summarized in the supplementary materials (Fig. S1; Table S1; Table S2).

The MANOVA test indicated a significant difference ($p < 0.05$) between Day 0 and Day 92 for all parameters reflecting soil conditions. This finding underscores the substantial transformation of SOM throughout a simulated vegetation period. Results revealed a consistent decline in SOC content, from 2.04 % (m/m) at Day 0–1.93 % (m/m) by Day 92, alongside a parallel reduction in the DOC/SOC ratio, which dropped from 4.35×10^{-4} to 2.61×10^{-4} (Fig. 2, Fig. S2). A strong temporal relationship between enzyme activities and SOM composition emerged. The aliphatic compounds in SOM decreased markedly, from 1.8 at Day 0–1.0 at the end of the simulated vegetation period. In contrast, aromatic compounds exhibited an initial increase from 5.86 to 7.13 at Day 14, stabilising at 6.55 by Day 92. The increase in aromatic compounds reflects the aromaticity index, which rose from 1.35 at Day 0–1.54 by Day 92. Enzyme activity displayed significant temporal variations linked to SOM dynamics. DHA enzyme activity assays are closely associated with SOC content ($r = 0.82$), declining from 78.95 mU/g at Day 0–17.77 mU/g by Day 92. In contrast, ACP activity demonstrated a gradual and sustained increase, from 0.03 mU/g at Day 0–0.046 mU/g by Day 92, showing a strong inverse correlation with SOC ($r = -0.94$). These patterns indicate that as SOC diminished, enzyme activity adjusts in the opposite direction. A strong temporal relationship between enzyme activity and SOM composition emerged. ACP activity has a positive correlation with time ($r = 0.99$); whereas, DHA exhibited an inverse trend (−0.70). Additionally, the DOC/SOC ratio, along with the aliphatic-to-aromatic compound ratio, significantly shifted over time. As the DOC/SOC ratio decreased (−0.99), the proportion of aliphatic compounds declined (−0.98), while the relative abundance of aromatic compounds increased with time ($r = 0.85$).

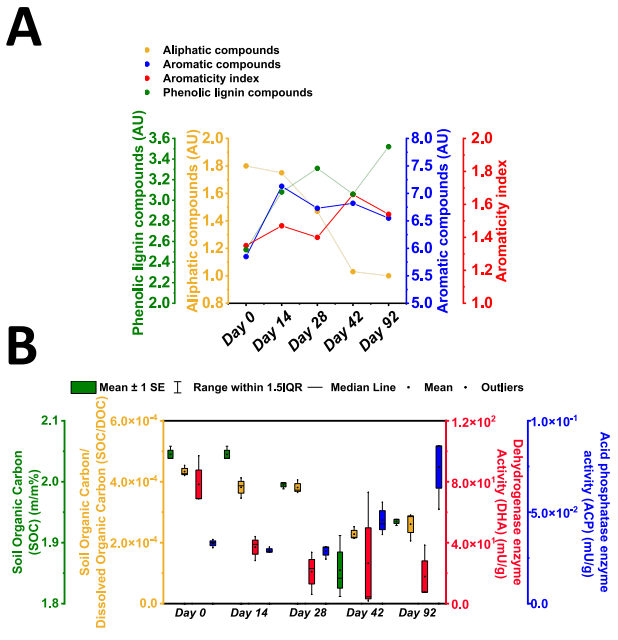


Fig. 2. Changes over time of components closely associated with modifications of soil organic matter A: Changes in soil organic carbon (SOC), dissolved organic carbon/soil organic carbon (DOC/SOC) ratio, dehydrogenase (DHA) and phosphatase enzyme (ACP) activity the measured on different sampling times (Day 0, Day 14, Day 28, Day 42 and Day 92). **B:** Absorbance intensities of aliphatic, aromatic and phenolic lignin components (based on FTIR spectra) indicated by the aromaticity index as a function of sampling times.

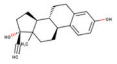
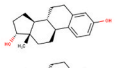
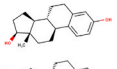
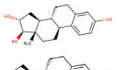
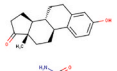
3.2. Evaluation of sorption behaviour of PhACs

Based on previous research (Szabó et al., 2024; Filep et al., 2021), we divided the investigated PhACs into two major competitive groups (CP1 and CP2), based on their physicochemical properties. We classified compounds according to their vdWSA and $\log_D$, highlighting differences in their physicochemical properties (Table 1). Group 1 (CP1) consisted of estrogens, such as EE2, E1, E3, BE2, and LE2, which are characterized by a $\log_D$ value of ≥2.66 and a vdWSA exceeding 429.56 Å^2. These compounds typically exhibit higher lipophilicity and larger molecular size. In contrast, Group 2 (CP2) included compounds with relatively (compared to CP1) lower $\log_D$ values and smaller vdWSA, such as DFC, 5HODFC, CBZ and TCBZ. These compounds are less lipophilic and have smaller molecular sizes. During incubation, no significant differences ($p > 0.05$) in pH values were observed across the sampling days, which allows us to exclude the effect of pH variation on the dissociable components. The following key parameters illustrate the main adsorption-desorption trends during the incubation period: the maximum adsorbed amount of PhACs (q_{max}, μg/g), saturation time (T_{sat}, min), and desorption percentage (Pd%, m/m) at Day 0 and Day 92 are highlighted in the text, as they best reflect the significant changes in the sorption dynamics as a function of time. In contrast, the results for the other sampling days (Nguyen et al., 2023; Wu et al., 2022; Kodešová et al., 2023) and the other parameters, such as breakthrough time ($T_{break,}$ min), area under adsorption curves ($A_{area,}$ min), total soil adsorption capacity ($q_{total,}$ μg), area under desorption curves (D_{area}, min) are presented (Table S3; Table S4).

At Day 0, the compounds in CP1 (i.e., estrogens) exhibited notably higher q_{max} values. For example, EE2 had a q_{max} of 1.31 μg/g, while BE2 showed an even higher value of 1.72 μg/g (Table S3). In contrast, the less hydrophobic and hydrophilic compounds in CP2 demonstrate lower initial adsorption capacities, such as DFC, with a q_{max} of 0.58 μg/g, and TCBZ, with 0.11 μg/g. Similarly, the key parameter T_{sat} representing the saturation time of the soil for each PhACs, was significantly ($p < 0.05$) longer for CP1 compounds with higher lipophilicity (EE2: 104.93 min, BE2: 105.58 min); whereas, CP2 compounds exhibited much shorter times (DFC: 29.62 min, TCBZ: 11.00 min). Despite belonging to CP2, 5HODFC displayed significantly ($p < 0.05$) different adsorption behaviour, with a T_{sat} of 97.21 min, much longer than other CP2 compounds. Its q_{max} value of 0.94 μg/g also indicated a higher adsorption affinity than other CP2 compounds, though still lower than those in CP1. The desorption patterns further highlight differences between the two groups. CP1 compounds showed lower desorption percentages, reflecting stronger binding: EE2 Pd% = 30.45 %, BE2 Pd% = 36.08 %, which mean the sorption processes are irreversible in the given conditions. In contrast, CP2 compounds exhibited desorption, which was reversible to a significant degree ($p < 0.05$): CBZ Pd% = 79.24 %, TCBZ Pd% = 86.25 %. However, 5HODFC displaying lower desorption (Pd% = 17.08 %) between the two CP characteristics.

By Day 92, a marked reduction in sorption was observed across both CP1 and CP2, with the previously significant differences in q_{max} between the two groups ($p < 0.05$), evident on Day 0, completely disappearing by the end of the incubation period. Comparisons could now only be made within the individual CPs themselves. In CP1, q_{max} values drastically declined, with EE2 q_{max} dropping to 0.09 μg/g and BE2 q_{max} to 0.08 μg/

Table 1
Chemical properties of PhACs calculated at soil pH 7.28, with competitive grouping based on physicochemical properties, primarily logD (pH-dependent lipophilicity) and vdWSA (van der Waals surface area) parameters.

	PhACs		logD	α_0[a]	α^-[b]	α_+[c]	nHBd[d]	nHBa[e]	nAliphatic bond	nAromatic bond	vdWSA[f]
Competitive group 1 (CP1)	EE2		**3.90**	99.7	0.3	0	2	2	19	6	**471.19**
	LE2		**3.74**	99.7	0.3	0	2	4	17	6	**436.59**
	BE2		**3.74**	99.7	0.3	0	2	4	17	6	**436.59**
	E3		**2.67**	99.7	0.3	0	3	6	18	6	**444.72**
	E1		**4.31**	99.7	0.3	0	1	4	17	6	**429.57**
Competitive group 2 (CP2)	CBZ		**2.77**	100	0	0	2	2	8	12	**321.86**
	TCBZ		**0.81**	100	0	0	4	6	10	12	**357.6**
	DFC		**0.92**	0.02	99.98	0	1	6	8	12	**363.47**
	5HODFC		**0.58**	0.01	99.9	0	1.99	8.01	9	12	**374.09**

[a] Fraction of PhAC as neutral form.; [b] Fraction of PhAC as positive form.; [c] Fraction of PhAC as negative form.;
[d] The number of hydrogen bond donor sites.; [e] The number of hydrogen bond acceptor sites.; [f] van der Waals surface area

g. CP2, on the other hand, exhibited near-complete depletion of sorption, with DFC q_{max} = 0.00 μg/g and TCBZ q_{max} = 0.01 μg/g. DFC remained entirely in the liquid phase by the end of the incubation period. In contrast, 5HODFC retained a relatively higher sorption capacity (q_{max} = 0.09 μg/g), aligning more closely with the sorption observed for CP1 compounds. T_{sat} values were also significantly ($p < 0.05$) reduced by Day 92. CP1 compounds exhibited shortened saturation times, with EE2 T_{sat} = 6.16 min and BE2 T_{sat} = 5.32 min. CP2 displayed similarly reduced T_{sat} values, particularly for CBZ (T_{sat} = 3.57 min) and TCBZ (T_{sat} = 3.14 min). DFC, having no adsorption, showed no measurable saturation (T_{sat} = 0.00 min). 5HODFC in CP2 displayed a notable T_{sat} value of 6.82 min, comparable to that of CP1 compounds. Desorption mechanisms had also shifted dramatically by Day 92. At the same time, CP1 became nearly fully desorbed by the end of the simulated vegetation period, indicating a near-complete loss of adsorption capacity. Desorption percentages for CP1 reached 100.00 % for EE2 and 100.00 % for BE2. In CP2, DFC showed no adsorption and, therefore, no desorption (Pd% = 0.00 %), while CBZ exhibited significantly ($p < 0.05$) increased mobility (Pd% = 91.90 %). 5HODFC continued deviating from this trend, with a lower desorption percentage (Pd% = 13.93 %) even at Day 92.

3.3. Evaluation of temporal changes of the sorption parameters through canonical variates

In this section, we further investigate how the previously described sorption parameters evolve over time through the use of Canonical Correlation Analysis (CCA). This approach is employed to identify which physicochemical parameters of PhACs dominate the sorption process and how this impact shifts over time across different sampling days. These associations are analyzed through canonical variables derived as linear combinations of the two variable groups (U and V). The first variable canonical variate set defined per sampling day (U, Eq. (1)) included sorption metrics such as T_{break}, T_{sat}, q_{max}, A_{area}, q_{total}, D_{area}, q_{dtotal}, and Pd % (Table S5). The second variable canonical variate group defined per sampling day (V, Eq. (2)) related to the physicochemical properties of PhACs, including pKa value, pH, log_D, nAlb/nArb, nHBA/nHBD and vdWSA (Table 1).

Four CCAs were performed on the data measured at Day 0–14 (014D1, 014D2), Day 28 (28D1, 28D2), Day 42 (42D1, 42D2), and Day 92 (92D1, 92D2) (Table S6). To ensure the viability of statistical analysis, the data from Day 0 and Day 14 were combined, as no significant differences ($p > 0.05$) were observed in the sorption data between these days (Table S3, Table S4). Significant canonical correlations were observed at Day 0–14, Day 28, and Day 92 intervals ($p < 0.01$), while no significant canonical correlation was found for Day 42 (42D1 $p < 0.07$; 42D2 $p < 0.65$). Therefore, Day 42 results were not evaluated chemometrically (Table S5).

The canonical correlations for the pairs of variates from 014D1 and 014D2 were significant ($p < 1.60 \times 10^{-7}$; $p < 4.00 \times 10^{-2}$), requiring simultaneous analysis (Table S6). The two key parameters indicating adsorption affinities, q_{max} (0.63) and q_{total} (1.20), exhibit a positive relationship with log_D (8.15) and vdWSA (4.61) in the 014D2 canonical correlation. Additionally, a similar positive relationship between T_{sat} (1.01), log_D (8.15), and vdWSA (4.61). CP1 display greater adsorption affinity during the early stages of the simulated vegetation period. This elevated sorption occurs in soils with higher SOM content (2.04 % m/m) and a higher DOC/SOC ratio (4.35×10^{-4}). In the 014D1 canonical correlation, a positive relationship was also identified between T_{break} (0.15) and parameters related to neutrality (neutral = 1.27). While the parameter for negativity is given by a canonical coefficient of −1.23, and the canonical correlation will be inversely related to the T_{break} (0.15). In terms of desorption dynamics, during the baseline period (Day 0–14), we observed an inverse relationship among log_D (8.15), vdWSA (4.61), nHBD (3.16), and nArb(3.16) with desorption parameters (D_{area} = −0.88; qd_{total} = −0.40; Pd (%) = −0.51) in the 014D2 canonical correlation between groups U and V. In the 014D1 canonical correlation, we found an inverse association between negativity (−1.23) and desorption parameters (D_{area} = 7.26; qd_{total} = 0.16; Pd (%) = 0.10), reflecting phenomena similar to those observed in 014D2, where negativity had a weight of 1.30 and desorption parameters were negatively weighted.

At Day 28, a significant shift ($p < 6.12 \times 10^{-8}$; $p < 1.00 \times 10^{-3}$) can be seen in the direction of relationships between the U and V sets in the canonical correlations 28D1 and 28D2, with a change in the sign of the correlations (Table S6). Nevertheless, the primary trends in the adsorption-desorption dynamics of CP1 and CP2 remains unchanged (Table S3; Table S4).

At Day 92, the canonical correlation analysis for the 92D1 variate revealed significant trends ($p < 4.33 \times 10^{-4}$; $p < 1.39 \times 10^{-2}$) between the U and V variable sets. The log_D parameter exhibited a negative coefficient (−9.15), while adsorption parameters such as q_{max} (538.26), T_{sat} (0.41), and q_{total} (5.91) were positive, indicating an inverse relationship between log_D and these adsorption metrics. Within the 92D1 canonical correlation, log_D (−9.15) was negatively associated; whereas, D_{area} (31.68) and Pd (%) (0.32) displayed positive coefficients, further confirming the inverse relationship among these variables. The 92D1 correlation revealed a direct relationship between negative charge (−2.77) and T_{break} (−20.49), as well as A_{area} (−4.44), indicating that under the altered adsorption conditions related to soil parameters, PhACs in CP2 will exhibit relatively greater adsorption affinity by Day 92, contrasting with the inverse relationship observed at Day 0. In contrast, the 92D2 variate demonstrated negative weighting for negativity (−0.53) and all desorption parameters ($D_{area} = -0.25$; $qd_{total} = -4.33$; Pd (%) = −0.84). Additionally, a positive correlation observed between negative charge (−0.53) and T_{break} (−3.15) within the 92D2 correlation. Thus, by Day 92, the altered soil properties substantially modify the adsorption-desorption processes of PhACs in CP2. Relative to their initial states, these compounds exhibit increased binding affinity.

3.4. Geometric (vectorial) CCA interpretation of the temporal changes in the adsorption and physicochemical parameters of PhACs with HCA

In the ordination biplots of CCA U-vectors and V-vectors on Day 0–14, axis one (Can 1) represents 86.63 % and axis two (Can 2) 6.25 % of the total variance. This means that in the exploration of relationships, the separation along the Can 1 axis has a large explanatory power ($p < 1.60 \times 10^{-7}$; $p < 4.00 \times 10^{-2}$). In the canonical space CP1 and CP2 are separated (Fig. 3). CP1 is mostly described by the adsorption vectors (T_{sat}, A_{area}, q_{total}, q_{max}), but there are also differences in the confidence interval within groups. E1 and E3 are already moving towards the desorption vectors (D_{area}). The CP2 compounds are positioned in the opposite direction to the sorption vectors, and 5HODFC is located far away from the other members of the group. In the V vectors biplot, the same trends occur e.g. CP1 and CP2 are distributed in two different directions. PhACs in CP1 are located at the direction of hydrophobic vectors such as log_D, number of Aliphatic bonds, neutrality, and vdWSA. While CP2 has shifted in the direction of negativity (especially 5HDFC), and the number of H bond donor/acceptor, and number of aromatic bonds. Based on HCA for the Day 0–14, two primary competitive partnerships were identified: CP1, consisting of EE2, E1, E3, BE2, and LE2, and CP2, comprising DFC, 5HODFC, CBZ, and TCBZ. Within these main clusters, further subdivisions were observed. In CP1, BE2, LE2, and EE2 clustered together; whereas, E1 and E3 formed a distinct subgroup. Similarly, within CP2, 5HODFC was isolated in a separate cluster, indicating a divergent behaviour compared to the other compounds in this group.

At Day 28, the Can 1 axis accounted for 62.24 % of the total variance, while the Can 2 axis explained 18.40 %. The divergence trend of the Can 1 axis between CP1 and CP2 remained consistent with that observed at Day 0–14 ($p < 6.12 \times 10^{-8}$; $p < 1.00 \times 10^{-3}$). However, there were noticeable changes in the magnitude and direction of the confidence intervals. Within the U vectors of CP1, not only did E3 and E1 move towards the desorption vectors (D_{area}, Pd%, q_{dtotal}), but BE2 and LE2 also followed a similar course. Meanwhile, EE2 and BE2 in CP1 were positioned towards the adsorption vectors (A_{area}, q_{max}, T_{sat}, q_{total}, T_{break}). In contrast, the confidence interval of CP2 decreased, indicating that 5HODFC no longer moved separately from the other compounds. Most of the vectors in CP2 were oriented along the Pd vector on the Can 2 axis. The V vectors' biplot displayed a similar trend to those seen at Day 0–14, with PhACs in CP1 predominantly positioned in the direction of vectors representing hydrophobicity. In contrast, CP2 shifted towards negative

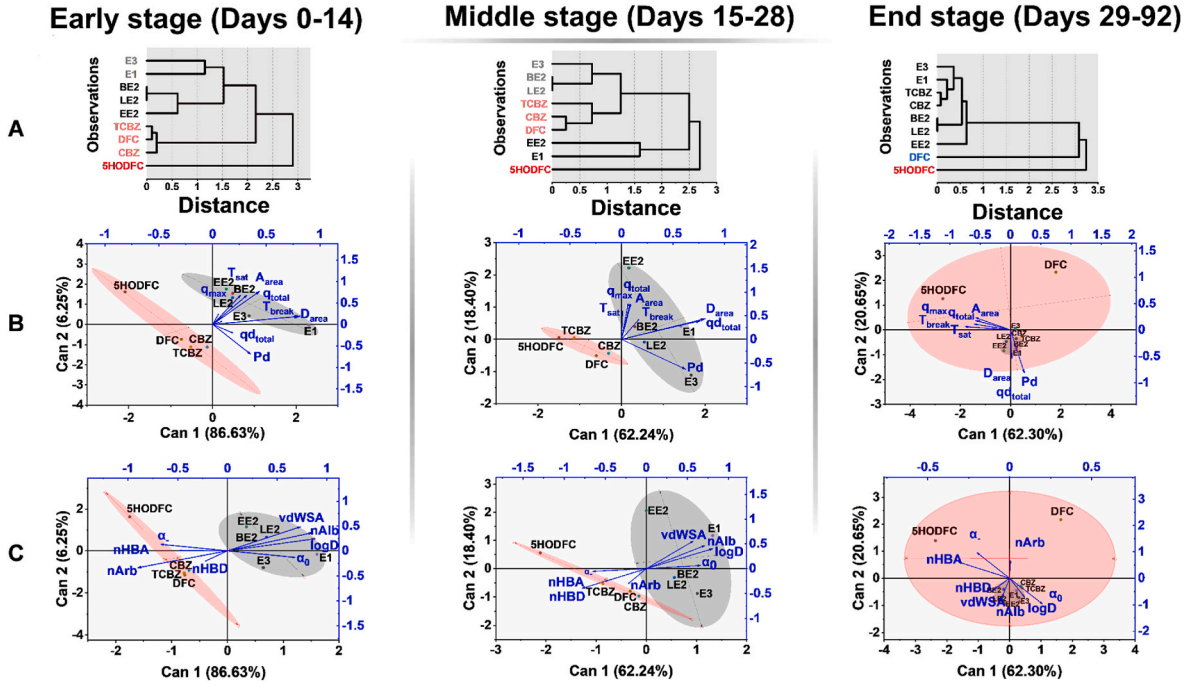


Fig. 3. Temporal evolution of the physicochemical properties and sorption dynamics of PhACs (CP1: grey, CP2: red) analyzed through Hierarchical Cluster Analysis (HCA) and geometric interpretation of Canonical Correlation Analysis (CCA). The early stage included the sampling time 1–2 (st1-2, day 0–14, the middle stage included st3 (day 28) and the end-stage corresponded to st5 (day 92). A: HCA with the sum of distances method with Euclidean distance as the metric abbreviations for specified PhACs **B:** The CCA results provided a geometric interpretation of time-dependent variations in the sorption dynamics of PhACs (CP1, CP2). **C:** The temporal evolution of physicochemical properties of PhACs.

values, especially with 5HODFC, and increased orientation towards the number of H-bond donors/acceptors and aromatic bonds. However, TCBZ, DFC, and CBZ began to move together and approached the CP1 confidence interval compared to Day 0–14.TheHCA analysis revealed changes in the two main competitive groups (clusters) from Day 0–14. Specifically, by Day 28, 5HODFC had moved markedly away from its original cluster (CP2) containing TCBZ, CBZ and DFC, and had effectively formed a separate cluster. Within CP1, EE2 and E1 started to diverge in the sorting space from LE2, BE2 and E3, forming a separate cluster on the dendrogram. As a result, the canonical space and the dendrogram at Day 28 indicated that the TCBZ, CBZ and DFC clusters started to move in the same direction as the cluster containing E3, BE2 and LE2, showing a convergent trend towards each other. Meanwhile, EE2 is moving into a cluster with E1 within the competitive partnership, and 5HODFC is forming a separate cluster.

The trend changes that have developed by Day 92 started in Day 42. At Day 92, the Can 1 axis of the CCA biplot explained 62.30 % of the total variance, while the Can 2 axis accounted for 20.65 %. By this time, the direction of the U vectors and the positions of the scores have completely changed. Similarly, the relative positions of the V vectors (as indicated by the cosine of the angles between them) show a significant shift ($p < 4.33 \times 10^{-4}$; $p < 1.39 \times 10^{-2}$). Among the U vectors, the PhACs belonging to CP1 were aligned towards those representing desorption, and the TCBZ and CBZ compounds from CP2 closely approached them in the canonical space. Consistent with this, the V vector biplot also revealed similar trends. However, in the case of physicochemical vectors, CBZ and TCBZ had not only approached but were already within the confidence interval of CP1. Among the U and V vectors, those representing hydrophobicity and desorption were aligned in the same direction, and all of CP1, along with CBZ and TCBZ from CP2, were grouped accordingly. In contrast, the negatively dissociating PhACs of CP2, 5HODFC and DFC, moved in the opposite direction at Day 92. Within the U vectors, these compounds were aligned in the direction of adsorption, while among the V vectors, they were positioned towards those indicating negative dissociation. Due to the departure of CBZ and TCBZ from CP2 to join CP1, the confidence interval of CP2 expanded significantly ($p < 4.33 \times 10^{-4}$; $p < 1.39 \times 10^{-2}$). As a result, the original sorption partnership dissolved.

4. Discussion

4.1. Soil organic matter transformation in the light of the enzyme activity

In a simulated vegetation period, we established the changes in OM quality and quantity without adding POM, as crops are also harvested from the fields at the end of the season. We examined the sorption behaviour of selected PhACs at five separate sampling times to investigate how changes in OM affected these processes. Changes in soil composition over time mirror the SOM decomposition described in the Soil Continuum Model (Lehmann and Kleber, 2015), showing a decrease in SOC as the soil microbial community utilizes OM as a nutrient. Enzyme activity displayed significant temporal variations linked to SOM dynamics. As the available larger, energy-rich components (e.g. carbohydrates, hydrocarbons) decreased, DHA activity decreased, making smaller, energy-depleted molecules. The pre-incubation procedure induced the Birch effect, i.e. a rapid increase in respiration (Xiang et al., 2008) as illustrated by the initial high levels of DHA enzyme, as remoistening the soil makes nutrients more available (Fig. 2/B). DHA enzymes play an important role in the oxidative degradation process of SOC by transferring hydrogen from substrate to acceptors. In line with our findings, Pascual et al. (2000) found that the activity of DHA decreases over time due to low SOM replenishment, which may be due to such factors as low levels of plant cover. The study of Kumar et al. (2013) also demonstrated a clear link between SOM and DHA enzyme levels. They found less DHA enzyme activity in the deeper layers of the soil compared to the OM-rich topsoils and enzyme activity was also lower in the cultivated area than in the non-tilled soils. This may be related to POM replenishment, as cultivated soils do not take up OM to the same extent as less disturbed soils. The ACP activity serves as a principal indicator of phosphorus cycling in soils. Its trend was opposite to DHA activity's, emphasizing these enzymes' distinct roles in carbon turnover. The increase in the ACP enzyme (Fig. 2/A) and the gradual decrease in POM can be explained by the fact that at the beginning of the experiment, there were still enough phosphorus compounds available for the microbes. However, as the Birch effect takes hold, the nutrients are constantly depleted due to the lack of POM replenishment. As available phosphorus compounds are used up, the microbial community aims to increase the amount of available phosphorus by boosting the ACP enzyme (Nannipieri et al., 2011; Wani, 2021; Azene et al., 2023). To achieve this, they begin to breakdown the phosphoester bonds of OM. The primary trend indicates a decrease in OM due to microbial activity, leading to reduced coverage of mineral phases that are usually coated with OM. This change results in the mineral surface playing a more significant role in adsorption compared to its role before the OM had decomposed. Due to the mineral composition of the investigated soil, there is a lack of minerals that would provide adsorption sites for PhACs, such as clay minerals, which have a large surface area (Table S2). Not only does the quantity of OM change during the incubation period, but it also undergoes a transformation, as indicated by the increase in aromatic components. The shift in the ratio indicates a transition to more recalcitrant forms of OM as decomposition progressed. The aliphatic systems are not only "depleted" but also transformed and condensed to form aromatic compounds by the microbial community (Wu et al., 2023; Niu et al., 2024). As activity increases, the amount of available aliphatics decreases, and the soil's aromaticity increases. A decrease in DOC/SOC balances this, since DOC is the part of SOC that is most easily available to SMC, responding more quickly to the processes occurring in the soil (Yang et al., 2021b; Zhang et al., 2024). The changes in OM indicate that the types and quantities of available functional groups have evolved during incubation, suggesting that sorption processes have been influenced as well. These patterns indicate that as SOC diminished, enzyme activity adjusts in the opposite direction. This decline mirrors the reduction in DHA, SOC content, and the ratio of aliphatic compounds, highlighting the shift from labile to more stable SOM formations as decomposition proceeded. In contrast, aromatic compounds became more prevalent over time and contribute to an increasing aromaticity index, indicating the system's transition towards more chemically stable compounds.

4.2. Temporal pattern of sorption processes

4.2.1. At the early stage of the simulated vegetation period

Alterations in soil composition over time can be tracked through changes in sorption parameters. Sorption processes depend mainly on the adsorbent's surface properties and the adsorbates' physicochemical properties. It was, therefore, necessary for CP1 and CP2 to differ in their properties, as then changes on the adsorbent surface could be immediately observed. Changes in surface properties, such as the number of adsorption sites (e.g. available functional groups), influenced the sorption parameters of PhACs. These can be monitored from the time variation of the main adsorption parameters of PhACs (e.g. q_{max}, T_{sat}, Pd%). The initial soil pH was 7.28, fluctuating only slightly during incubation (7.11–7.42), so that PhAC dissociation was not affected. CP1 compounds with higher hydrophobicity and lipophilicity were initially less mobile at the beginning of the simulated vegetation period. Conversely, CP2 displayed faster and more limited adsorption, which led to significantly higher desorption rates of 80–90 % than those observed in CP1. The exception to this trend was 5HODFC, suggesting alternative (third-way) binding mechanisms. Based on the logD value, 5HODFC is the most water-soluble compound among the investigated PhACs, indicating unexpectedly high adsorption affinity in the results. Consequently, the fundamental classification of PhACs by hydrophobic properties

proposed in the literature (Nguyen et al., 2023; Filep et al., 2021; Hong et al., 2023; El Brahmi et al., 2024) may not fully capture their behaviour in the soil–solution system. However, our initial groupings were supported by HCA and the fact that PhACs in the same group within canonical space occupied the same area; specifically, they had the same vectors pointing towards them. In CP1, estrogens have a great ability to form hydrogen bonds with the moieties of SOM (Ahmed et al., 2016). Due to their high vdWSA, they can also form layers on top of each other with hydrophobic interactions, which explains their high adsorption affinity. Like the estrogens, the combination of CBZ and TCBZ is hydrophobic but has a low vdWSA, which reduces the extent of adsorption. CBZ has only four H-bond sites, which limits the formation of H-bonds (Filep et al., 2021). This limitation explains why CBZ, TCBZ, DFC and 5HODFC have been grouped together. DFC and 5HODFC were fully dissociated at soil pH (7.11–7.42). Their adsorption was limited compared to CP1 due to their negative charge. 5HODFC has very similar sorption values to estrogens, but its desorption is even lower than that of CP1 members, only 17 %, which means mainly irreversible adsorption/non-linear adsorption. The larger number of hydrogen bond acceptor sites allows 5HODFC to form more specific interactions along hydrogen bonds with the surface of soil particles, e.g. hydroxyl groups (-OH) or amine groups (-NH_2). Especially in competitive systems, components with more nHBa compete more effectively for adsorption sites (Li et al., 2023). Despite the soil's negative pH charge, strong interactions may prevail in adsorption rather than the repulsive forces between the negatively charged soil particles and 5HODFC. In addition to the strong interactions of estrogens, hydrophobic interactions also play a significant role. This refers to the ability to form secondary bonds with non-polar groups in OM, such as alkyl chains (Thiele-Bruhn et al., 2004). These interactions are similarly applicable to CBZ and TCBZ within the CP2 group.

The results support the notion that PhACs with higher lipophilicity and larger molecular size, such as CP1 compounds (e.g., estrogens), display greater adsorption affinity during the early stages of the simulated vegetation period. This elevated sorption occurs in soils with higher SOM content and a higher DOC/SOC ratio (Table S1), indicating a higher proportion of labile OM and a lower SOM aromaticity index, reflecting a POM-rich initial environment. In contrast, dissociative compounds (e.g., DFC in CP2) will exhibit higher desorption activity, particularly when the soil's SOM content and labile carbon levels are higher in the initial phase.

4.2.2. At the middle stage of the simulated vegetation period

As we progress through the simulated vegetation period to Day 28, the primary sorption trends remain similar, but there is a shift in the direction of the relationships. Due to the physicochemical properties of PhACs, what were minor differences between the compounds become increasingly noticeable. As OM gradually decreased, CBZ, TCBZ, and DFC began to move together within CP2, with some members of CP1 also starting to align with the compounds in the CP2 group. The number of potential adsorption sites also declines, which reduces the amount of polar functional groups (-OH, -COOH) that can form strong hydrogen bonds with PhACs. At this point, the remaining sites are already subject to competition, and therefore not only 5HODFC but also EE2 are significantly separated, because their properties allow them to form hydrogen bonds primarily. The other components, e.g. E3, LE3, can form less strong interactions, so their desorbed amount will be higher, indicating reduced retention. Overall, this subtle change in the sorption behaviour, resulting from a concurrent decrease in soil SOM content and a reduction in labile carbon within the DOC/SOC ratio, is accompanied by an increase in the proportion of aromatic compounds and a decrease in aliphatic compounds.

4.2.3. At the end stage of the simulated vegetation period

By Day 92, significant changes were already apparent. Different physicochemical parameters influence the end stage of the simulated vegetation period than at the start of incubation. The soil's retention of PhACs decreased compared to the initial stage, which is related to a decrease in SOM. The trend suggests that for dissociating PhACs in CP2, such as negatively charged ionic components, a decrease in SOM and an increase in the available mineral surface area led to a higher adsorption rate and a lower desorption rate. This interpretation has limitations, as DFC should have shown a similar trend. Previous work (Filep et al., 2021) reported that mineral surfaces caused increased retention of ionic PhACs in soils with lower OM content. The novelty of the case is the finding that the reduction in the number of available functional groups from OM, combined with the competition among PhACs, results in a lower extent of adsorption of PhACs. Consequently, PhACs with more "favourable" properties, for example in their ability to displace DFC, tend to dominate over others. Consequently, even in cases where the amount of OM decreases, SOM-dominated adsorption remains a consistent phenomenon.

Once PhACs enter soils they can undergo transformations through biotic or abiotic reactions (Nguyen et al., 2021), and, as a consequence, degradation products can form. In the case of 5HODFC, it is more stable, toxic, and persistent than the parent compound (DFC), which causes accumulation in the tilled layer throughout the vegetation period. In our study, the behaviour of CBZ and TCBZ was consistent during incubation, with similar sorption dynamics observable in the parent compound (CBZ) and the degradation product (TCBZ), as well as in estrogens. Their common feature is hydrophobicity, where the presence of hydrophobic PhACs uniformly results in their reduced soil retention towards the end of the simulated vegetation period due to OM transformation. In contrast, large differences can be found between dissociating compounds. If these dissociating PhACs are able to interact not only with Coulomb forces but also with stronger hydrogen bonds, they will play a more prominent role in adsorption, such as 5HODFC. By the end of the vegetation period, the soil retention strength for PhACs will primarily be determined by the ratio of nHBa to nHBd. Indeed, hydrogen bonds can form with OM and functional groups of mineral particles. The HCA also shows that the original competitive grouping has disappeared by this stage. Due to their hydrophobic properties, the estrogens have formed a new competitive group with CBZ and TCBZ. Meanwhile, the two dissociating PhACs have completely separated, with 5HODFC becoming mostly irreversible, while DFC did not adsorb. At the closure of the simulated vegetation period, the PhACs that continued to adsorb to the remaining components of OM were those capable of forming a significant number of H-bonds. In light of these novel findings, the nHBda ratio emerges as a critical factor to consider when assessing the persistence of organic micropollutants.

This integrated approach, combining parent pharmaceuticals with their most common metabolites under continuous incubation and explicitly considering the dynamic nature of SOM, has not previously been addressed. The findings demonstrate that even within a single vegetation period, adsorption–desorption dynamics can undergo substantial shifts, offering a novel perspective on contaminant–soil interactions.

5. Conclusion

During the investigation of the Mollisol's adsorption properties, the area without POM supply is always a snapshot of a given SOM quality and quantity. At every time point, as a function of the transformation of SOM, the sorption of PhACs is driven by a different physicochemical property, e.g., hydrophobicity, negativity, or ratio of nHBda. Microchanges in the OM can completely rewrite the adsorption dynamics, and qualitative changes can influence which properties of the PhACs will control the sorption processes. Many studies indicate that soils with low OM content are primarily characterized by mineral-dominated adsorption. In our study, it appears that the entire sorption process is influenced by SOM, even when its amount is considerably reduced. The timing of soil sampling for measuring organic micropollutants can

significantly influence the results, as it is closely linked to the specific stage of the vegetation period when samples are collected. Since the transformation rate of SOM varies throughout these stages, this variation directly affects the medium's retention capacity. In our view, this study addresses a gap by considering multiple time points within a single vegetation cycle to assess the behaviour of PhACs and their degradation products in Mollisols, a soil type that accounts for approximately one-fifth of all agricultural land. Our findings highlight that these compounds exhibit highly dynamic mobility in arable Mollisols, independent of their parent compound, which has significant implications for their terrestrial and agricultural availability. This temporal variability suggests that their retention, mobility, and associated risks fluctuate continuously throughout the vegetation period, emphasizing the need for time-sensitive risk assessments in agroecosystems. While the present work focuses on a single vegetation period, it opens the way for future studies to test the observed mechanisms under broader environmental conditions.

CRediT authorship contribution statement

Lili Szabó: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Zoltán Szalai:** Writing – review & editing, Funding acquisition, Conceptualization. **Attila Csaba Kondor:** Writing – review & editing, Funding acquisition. **Anna Vancsik:** Visualization. **Balázs Vajna:** Methodology, Investigation, Funding acquisition. **Csaba László Maller:** Methodology, Investigation. **Csilla Király:** Methodology. **Zoltán Dévény:** Visualization, Map visualization, Soil data analysis, Review & editing. **Bruna Silva:** Writing – review & editing, Supervision. **Colin A. Booth:** Writing – review & editing. **László Bauer:** Writing – review & editing, Writing – original draft, Visualization, Software, Investigation, Formal analysis, Data curation.

Generative AI and figures, images and artwork

No generative AI or AI-assisted tools were used to create or modify any images, figures, or artwork in the submitted manuscript.

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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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jenvman.2025.127492.

Data availability

All data are available in the supplementary materials and in the data repository at the link below: https://repo.researchdata.hu/dataset.xhtml;jsessionid=09918ec6c30bb5f6f3aac4aafd4a?persistentId=hdl%3A21.15109%2FARP%2FPNRMZT&version=DRAFT.

References

Ahmed, A.A., Thiele-Bruhn, S., Leinweber, P., Kühn, O., 2016. Towards a molecular level understanding of the sulfanilamide-soil organic matter-interaction. Sci. Total Environ. 559, 347–355. https://doi.org/10.1016/j.scitotenv.2016.03.136.

Alhalabi, A.M., Meetani, M.A., Shabib, A., Maraqa, M.A., 2024. Sorption of pharmaceutically active compounds to soils: a review. Environ. Sci. Eur. https://doi.org/10.1186/s12302-024-00984-9.

Ambrózy, Z., 'Juhász Á, P., Marosi, S., Dövényi, 2010. Inventory of Microregions in Hungary 876. Budapest. http://real.mtak.hu/id/eprint/1416.

Azene, B., Zhu, R., Pan, K., Sun, X., Nigussie, Y., Gruba, P., Raza, A., Guadie, A., Wu, X., Zhang, L., 2023. Land use change alters phosphatase enzyme activity and phosphatase-harboring microbial abundance in the subalpine ecosystem of southeastern Qinghai-Tibet Plateau, China. Ecol. Indic. 153. https://doi.org/10.1016/j.ecolind.2023.110416.

Bauer, L., Szalai, Z., Vancsik, A., Kondor, A.C., Dévény, Z., Silva, B., Szabó, L., 2025. Thermodynamic modelling of pharmaceutical sorption in soil systems: a comparative study of batch and fixed-bed approaches. Ecotoxicol. Environ. Saf. 302, 118640. https://doi.org/10.1016/j.ecoenv.2025.118640.

Canteral, K.F.F., Vicentini, M.E., de Lucena, W.B., de Moraes, M.L.T., Montanari, R., Ferraudo, A.S., Peruzzi, N.J., La Scala, N., Panosso, A.R., 2023. Machine learning for prediction of soil CO2 emission in tropical forests in the Brazilian Cerrado. Environ. Sci. Pollut. Control Ser. 30, 61052–61071. https://doi.org/10.1007/s11356-023-26824-6.

Carter, L.J., Harris, E., Williams, M., Ryan, J.J., Kookana, R.S., Boxall, A.B.A., 2014. Fate and uptake of pharmaceuticals in soil–plant systems. J. Agric. Food Chem. 62, 816–825. https://doi.org/10.1021/jf404282y.

Chen, J., Luo, Y., van Groenigen, K.J., Hungate, B.A., Cao, J., Zhou, X., Wang, R., 2018. A keystone microbial enzyme for nitrogen control of soil carbon storage. Sci. Adv. 4. https://doi.org/10.1126/sciadv.aaq1689.

Cuthbert, R., Taggart, M.A., Prakash, V., Saini, M., Swarup, D., Upreti, S., Mateo, R., Chakraborty, S.S., Deori, P., Green, R.E., 2011. Effectiveness of action in India to reduce exposure of gyps vultures to the toxic veterinary drug diclofenac. PLoS One 6, e19069. https://doi.org/10.1371/journal.pone.0019069.

Demyan, M.S., Rasche, F., Schulz, E., Breulmann, M., Müller, T., Cadisch, G., 2012. Use of specific peaks obtained by diffuse reflectance Fourier transform mid-infrared spectroscopy to study the composition of organic matter in a Haplic Chernozem. Eur. J. Soil Sci. 63, 189–199. https://doi.org/10.1111/j.1365-2389.2011.01420.x.

El Brahmi, A., Azzellino, A., Malpei, F., Buttiglieri, G., 2024. Are membrane bioreactors really more efficient in removing pharmaceutical substances?—Variance component analysis of micropollutant removal. Water, Air, Soil Pollut. 235. https://doi.org/10.1007/s11270-024-07505-7.

Erdel, E., Şimşek, U., Kesimci, T.G., 2023. Effects of fungi on soil organic carbon and soil enzyme activity under agricultural and pasture land of Eastern Türkiye. Sustainability 15, 1765. https://doi.org/10.3390/su15031765.

Estevez, E., Hernandez-Moreno, J.M., Fernandez-Vera, J.R., Palacios-Diaz, M.P., 2014. Ibuprofen adsorption in four agricultural volcanic soils. Sci. Total Environ. 468–469, 406–414. https://doi.org/10.1016/j.scitotenv.2013.07.068.

Fenet, H., Mathieu, O., Mahjoub, O., Li, Z., Hillaire-Buys, D., Casellas, C., Gomez, E., 2012. Carbamazepine, carbamazepine epoxide and dihydroxycarbamazepine sorption to soil and occurrence in a wastewater reuse site in Tunisia. Chemosphere 88, 49–54. https://doi.org/10.1016/j.chemosphere.2012.02.050.

Filep, T., Szabó, L., Kondor, A.C., Jakab, G., Szalai, Z., 2021. Evaluation of the effect of the intrinsic chemical properties of pharmaceutically active compounds (PhACs) on sorption behaviour in soils and goethite. Ecotoxicol. Environ. Saf. 215, 112120. https://doi.org/10.1016/j.ecoenv.2021.112120.

Filep, T., Zacháry, D., Kovács, A.B., Király, C., Béni, Á., Jakab, G., Juhász, E.K., Szalai, Z., 2024. Insight into the dynamics of protected and non-protected carbon pools in four

soils with different land uses. Plant Soil. https://doi.org/10.1007/s11104-024-07054-2.
Food and Agriculture Organization of the United Nations (FAO). FAO–UNESCO soil map of the world. https://www.fao.org/soils-portal/data-hub/soil-maps-and-databases/faounesco-soil-map-of-the-world/en/. (Accessed 15 January 2025).
Franklin, A.M., Williams, C., Andrews, D.M., Watson, J.E., 2022. Sorption and desorption behavior of four antibiotics at concentrations simulating wastewater reuse in agricultural and forested soils. Chemosphere 289, 133038. https://doi.org/10.1016/j.chemosphere.2021.133038.
Graouer-Bacart, M., Sayen, S., Guillon, E., 2016. Adsorption and co-adsorption of diclofenac and Cu(II) on calcareous soils. Ecotoxicol. Environ. Saf. 124, 386–392. https://doi.org/10.1016/j.ecoenv.2015.11.010.
Gresina, F., 2020. Comparison of pipette method and state of the art analytical techniques to determine granulometric properties of sediments and soils. Hungarian Geographical Bulletin 69, 27–39. https://doi.org/10.15201/hungeobull.69.1.3.
Hickey, W.J., Parthipan, P., Cheng, L., Karthikeyan, P., Rahman, P.K.S.M., 2024. Editorial: biosurfactants - next-generation biomolecules for enhanced biodegradation of organic pollutants. Microbiotechnology II. https://doi.org/10.3389/fmicb.2024.1513087.
Hong, H., Liu, C., Li, Z., 2023. Chemistry of soil-type dependent soil matrices and its influence on behaviors of pharmaceutical compounds (PCs) in soils. Heliyon 9 (12), 1. https://doi.org/10.1016/j.heliyon.2023.e22931.
Jelic, A., Gros, M., Ginebreda, A., Cespedes-Sánchez, R., Ventura, F., Petrovic, M., Barcelo, D., 2011. Occurrence, partition and removal of pharmaceuticals in sewage water and sludge during wastewater treatment. Water Res. 45, 1165–1176. https://doi.org/10.1016/j.watres.2010.11.010.
Kodešová, R., Grabic, R., Kočárek, M., Klement, A., Golovko, O., Fér, M., Nikodem, A., Jakšík, O., 2015. Pharmaceuticals' sorptions relative to properties of thirteen different soils. Sci. Total Environ. 511, 435–443. https://doi.org/10.1016/j.scitotenv.2014.12.088.
Kodešová, R., Fedorova, G., Kodeš, V., Kočárek, M., Rieznyk, O., Fér, M., Švecová, H., Klement, A., Bořík, A., Nikodem, A., Grabic, R., 2023. Assessment of potential mobility of selected micropollutants in agricultural soils of the Czech Republic using their sorption predicted from soil properties. Sci. Total Environ. 865, 161174. https://doi.org/10.1016/j.scitotenv.2022.161174.
Kumar, S., Chaudhuri, S., Maiti, S.K., 2013. Soil dehydrogenase enzyme activity in natural and mine soil - a review. Middle East J. Sci. Res. 13 (7), 898–906. https://doi.org/10.5829/idosi.mejsr.2013.13.7.2801.
Lal, R., 2020. Soil organic matter and water retention. Agron. J. 112, 3265–3277. https://doi.org/10.1002/agj2.20282.
Lehmann, J., Kleber, M., 2015. The contentious nature of soil organic matter. Nature 528, 60–68. https://doi.org/10.1038/nature16069.
Lehmann, J., Solomon, D., 2010. Organic carbon chemistry in soils observed by synchrotron-based spectroscopy. Dev. Soil Sci. 289–312. https://doi.org/10.1016/S0166-2481(10)34010-4.
Li, J., Wen, Y., Li, X., Li, Y., Yang, X., Lin, Z., Song, Z., Cooper, J.M., Zhao, B., 2018. Soil labile organic carbon fractions and soil organic carbon stocks as affected by long-term organic and mineral fertilization regimes in the North China Plain. Soil Tillage Res. 175, 281–290. https://doi.org/10.1016/j.still.2017.08.008.
Li, N., Liu, Y., Du, C., Wang, Y., Wang, L., Li, X., 2023. A novel role of various hydrogen bonds in adsorption, desorption and co-adsorption of PPCPs on corn straw-derived biochars. Sci. Total Environ. 861. https://doi.org/10.1016/j.scitotenv.2022.160623.
Martínez-Alcalá, I., Pellicer-Martínez, F., Fernández-López, C., 2018a. Pharmaceutical grey water footprint: accounting, influence of wastewater treatment plants and implications of the reuse. Water Res. 135, 278–287. https://doi.org/10.1016/j.watres.2018.02.033.
Martínez-Alcalá, I., Pellicer-Martínez, F., Fernández-López, C., 2018b. Pharmaceutical grey water footprint: accounting, influence of wastewater treatment plants and implications of the reuse. Water Res. 135, 278–287. https://doi.org/10.1016/j.watres.2018.02.033.
Mejías, C., Martín, J., Santos, J.L., Aparicio, I., Alonso, E., 2021. Occurrence of pharmaceuticals and their metabolites in sewage sludge and soil: a review on their distribution and environmental risk assessment. Trends in Environmental Analytical Chemistry 30, e00125. https://doi.org/10.1016/j.teac.2021.e00125.
Mohd Razali, N., Bee Wah, Y., 2011. Power comparisons of Shapiro-Wilk, Kolmogorov-Smirnov. Lilliefors and Anderson-Darling Tests Journal of Statistical Modeling and Analytics 2 (1), 21–33. https://doi.org/10.13140/RG.2.1.1184.6647.
Morugán-Coronado, A., García-Orenes, F., Mataix-Solera, J., Arcenegui, V., Mataix-Beneyto, J., 2011. Short-term effects of treated wastewater irrigation on Mediterranean calcareous soil. Soil Tillage Res. 112, 18–26. https://doi.org/10.1016/j.still.2010.11.004.
Mrabet, R., Saber, N., El-Brahli, A., Lahlou, S., Bessam, F., 2001. Total, particulate organic matter and structural stability of a Calcixeroll soil under different wheat rotations and tillage systems in a semiarid area of Morocco. Soil Tillage Res. 57, 225–235. https://doi.org/10.1016/S0167-1987(00)00180-X.
Mrozik, W., Stefańska, J., 2014. Adsorption and biodegradation of antidiabetic pharmaceuticals in soils. Chemosphere 95, 281–288. https://doi.org/10.1016/j.chemosphere.2013.09.012.
Nannipieri, P., Giagnoni, L., Landi, L., Renella, G., 2011. Role of phosphatase enzymes in soil. Phosphorus in Action 215–243. https://doi.org/10.1007/978-3-642-15271-9_9, 2010.
Nguyen, P.Y., Carvalho, G., Reis, M.A.M., Oehmen, A., 2021. A review of the biotransformations of priority pharmaceuticals in biological wastewater treatment processes. Water Res. 188. https://doi.org/10.1016/j.watres.2020.116446.
Nguyen, M.-K., Lin, C., Nguyen, H.-L., Hung, N.T.Q., La, D.D., Nguyen, X.H., Chang, S.W., Chung, W.J., Nguyen, D.D., 2023. Occurrence, fate, and potential risk of pharmaceutical pollutants in agriculture: challenges and environmentally friendly solutions. Sci. Total Environ. 899, 165323. https://doi.org/10.1016/j.scitotenv.2023.165323.
Niu, Y., Li, Y., Lou, M., Cheng, Z., Ma, R., Guo, H., Zhou, J., Jia, H., Fan, L., Wang, T., 2024. Microbial transformation mechanisms of particulate organic carbon to mineral-associated organic carbon at the chemical molecular level: highlighting the effects of ambient temperature and soil moisture. Soil Biol. Biochem. 195. https://doi.org/10.1016/j.soilbio.2024.109454.
Ojobe, B., Zouzelka, R., Satkova, B., Vagnerova, M., Nemeskalova, A., Kuchar, M., Bartacek, J., Rathousky, J., 2021. Photocatalytic removal of pharmaceuticals from greywater. Catalysts 11. https://doi.org/10.3390/catal11091125.
Pascual, J.A., Garcia, C., Hernandez, T., Moreno, J.L., Ros, M., 2000. Soil microbial activity as a biomarker of degradation and remediation processes. Soil Biol. Biochem. 1877–1883. https://doi.org/10.1016/S0038-0717(00)00161-9.
Patel, H., 2022. Comparison of batch and fixed bed column adsorption: a critical review. Int. J. Environ. Sci. Technol. 19, 10409–10426. https://doi.org/10.1007/s13762-021-03492-y.
Paudel, K., Amano, T., Acharya, R., Chaudhary, A., Baral, H.S., Bhusal, K.P., Chaudhary, I.P., Green, R.E., Cuthbert, R.J., Gallingan, T.H., 2016. Population trends in Himalayan Griffon in Upper Mustang, Nepal, before and after the ban on diclofenac. Bird. Conserv. Int. 26, 286–292. https://doi.org/10.1017/S0959270915000192.
Qiang, L., Cheng, J., Yi, J., Rotchell, J.M., Zhu, X., Zhou, J., 2016. Environmental concentration of carbamazepine accelerates fish embryonic development and disturbs larvae behavior. Ecotoxicology 25, 1426–1437. https://doi.org/10.1007/s10646-016-1694-y.
Qin, Q., Chen, X., Zhuang, J., 2017. The surface-pore integrated effect of soil organic matter on retention and transport of pharmaceuticals and personal care products in soils. Sci. Total Environ. 599–600, 42–49. https://doi.org/10.1016/j.scitotenv.2017.04.148.
Ramanayaka, S., Vithanage, M., Zhang, H., Semple, K.T., 2023. Role of soil organic matter on the retention and mobility of common plastic additives, Di(2-ethylhexyl) phthalate, bisphenol A and benzophenone, in soil. Environ. Res. 236, 116725. https://doi.org/10.1016/j.envres.2023.116725.
Schneider, U.A., Havlík, P., Schmid, E., Valin, H., Mosnier, A., Obersteiner, M., Böttcher, H., Skalský, R., Balkovič, J., Sauer, T., Fritz, S., 2011. Impacts of population growth, economic development, and technical change on global food production and consumption. Agric. Syst. 204–215. https://doi.org/10.1016/j.agsy.2010.11.003.
Shang, Z.C., Zhang, L.L., Wu, Z.J., Gong, P., Li, D.P., Zhu, P., Gao, H.J., 2012. The activity and kinetic parameters of oxidoreductases in phaeozem in response to long-term fertiliser management. J. Soil Sci. Plant Nutr. 597–607. https://doi.org/10.4067/S0718-95162012005000019.
Szabó, L., Vancsik, A., Király, C., Ringer, M., Kondor, A., Jakab, G., Szalai, Z., Filep, T., 2020. Investigation of the sorption of 17α-ethynylestradiol (EE2) on soils formed under aerobic and anaerobic conditions. Chemosphere 240, 124817. https://doi.org/10.1016/j.chemosphere.2019.124817.
Szabó, L., Vancsik, A., Bauer, L., Jakab, G., Király, C., Hatvani, I.G., Kondor, A.C., Szalai, Z., 2024. Effects of root-derived organic acids on sorption of pharmaceutically active compounds in sandy topsoil. Chemosphere 355, 141759. https://doi.org/10.1016/j.chemosphere.2024.141759.
Thiele-Bruhn, S., Seibicke, T., Schulten, H.-R., Leinweber, P., 2004. Sorption of sulfonamide pharmaceutical antibiotics on whole soils and particle-size fractions. J. Environ. Qual. https://doi.org/10.2134/jeq2004.1331.
Trumbore, S.E., 1997. Potential responses of soil organic carbon to global environmental change. Proc. Natl. Acad. Sci. 94, 8284–8291. https://doi.org/10.1073/pnas.94.16.8284.
Vancsik, A., Szabó, L., Bauer, L., Pirger, Z., Karlik, M., Kondor, A.C., Jakab, G., Szalai, Z., 2024. Impact of land use-induced soil heterogeneity on the adsorption of fluoroquinolone antibiotics, tested on organic matter pools. J. Hazard Mater. 474, 134704. https://doi.org/10.1016/j.jhazmat.2024.134704.
Veum, K.S., Goyne, K.W., Kremer, R.J., Miles, R.J., Sudduth, K.A., 2014. Biological indicators of soil quality and soil organic matter characteristics in an agricultural management continuum. Biogeochemistry 117, 81–99. https://doi.org/10.1007/s10533-013-9868-7.
Wang, X., Sheng, L., Li, Y., Jiang, H., Lv, Z., Qi, W., Luo, W., 2022. Soil labile organic carbon indicating seasonal dynamics of soil organic carbon in northeast peatland. Ecol. Indic. 138. https://doi.org/10.1016/j.ecolind.2022.108847.
Wani, S.A., 2021. Assessment of changes in soil organic carbon fractions and enzyme activities under apple growing ecosystems in temperate North-Western Himalayas. Resources, Environment and Sustainability 6. https://doi.org/10.1016/j.resenv.2021.100036.
Westhof, L., Köster, S., Reich, M., 2016. Occurrence of micropollutants in the wastewater streams of cruise ships. Emerging Contam. 2, 178–184. https://doi.org/10.1016/j.emcon.2016.10.001.
Wu, J., Lu, J., Wu, J., 2022. Adsorption and desorption of steroid hormones on saline soil. Front. Environ. Sci. Eng. 16, 140. https://doi.org/10.1007/s11783-022-1575-y.
Wu, D., Ren, C., Ren, D., Tian, Y., Li, Y., Wu, C., Li, Q., 2023. New insights into carbon mineralization in tropical paddy soil under land use conversion: coupled roles of soil microbial community, metabolism, and dissolved organic matter chemodiversity. Geoderma 432. https://doi.org/10.1016/j.geoderma.2023.116393.
Xiang, S.R., Doyle, A., Holden, P.A., Schimel, J.P., 2008. Drying and rewetting effects on C and N mineralization and microbial activity in surface and subsurface California grassland soils. Soil Biol. Biochem. 40, 2281–2289. https://doi.org/10.1016/j.soilbio.2008.05.004.

Yakutina, O.P., Nechaeva, T.V., Smirnova, N.V., 2015. Consequences of snowmelt erosion: soil fertility, productivity and quality of wheat on Greyzemic Phaeozem in the south of West Siberia. Agric. Ecosyst. Environ. 200, 88–93. https://doi.org/10.1016/j.agee.2014.10.021.

Yan, Q., Min, J., Yu, Y., Zhu, Z., Feng, G., 2017. Microbial community response during the treatment of pharmaceutically active compounds (PhACs) in constructed wetland mesocosms. Chemosphere 186, 823–831. https://doi.org/10.1016/j.chemosphere.2017.08.064.

Yang, X., Meng, J., Lan, Y., Chen, W., Yang, T., Yuan, J., Liu, S., Han, J., 2017. Effects of maize stover and its biochar on soil CO2 emissions and labile organic carbon fractions in Northeast China. Agric. Ecosyst. Environ. 240, 24–31. https://doi.org/10.1016/j.agee.2017.02.001.

Yang, Y., Liu, H., Dai, Y., Tian, H., Zhou, W., Lv, J., 2021a. Soil organic carbon transformation and dynamics of microorganisms under different organic amendments. Sci. Total Environ. 750, 141719. https://doi.org/10.1016/j.scitotenv.2020.141719.

Yang, Y., Liu, H., Dai, Y., Tian, H., Zhou, W., Lv, J., 2021b. Soil organic carbon transformation and dynamics of microorganisms under different organic amendments. Sci. Total Environ. 750. https://doi.org/10.1016/j.scitotenv.2020.141719.

Zhang, W., Tang, X., Thiele-Bruhn, S., 2021. Interaction of pig manure-derived dissolved organic matter with soil affects sorption of sulfadiazine, caffeine and atenolol pharmaceuticals. Environ. Geochem. Health 43, 4299–4313. https://doi.org/10.1007/s10653-021-00904-3.

Zhang, W., Tang, X., Chefetz, B., Thiele-Bruhn, S., 2024. Size and polarity fractions of mobile organic matter from manure affect the sorption of sulfadiazine, caffeine and atenolol in soil. J. Hazard Mater. 477. https://doi.org/10.1016/j.jhazmat.2024.135277.