Microchemical Journal 210 (2025) 112958

Contents lists available at ScienceDirect

Microchemical Journal

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

Review Article

Polyethersulfone potential in single and dual-phase passive samplers: A review

Henry MacKeown, Chiara Scapuzzi, Barbara Benedetti, Marina Di Carro, Emanuele Magi *

Department of Chemistry and Industrial Chemistry, University of Genoa, via Dodecaneso, 31 16146 Genoa, Italy

ARTICLE INFO

Keywords:
Passive sampling
Sampling rate
Partition coefficient
Membrane
POCIS
Polyethersulfone
Water monitoring

ABSTRACT

Single-phase passive samplers are often employed for the sampling of hydrophobic compounds in aqueous matrices. Recently, polyethersulfone (PES) has been proposed for integrative passive sampling of mid-polar compounds as an alternative to the more traditionally used polymers. However, dual-phase passive samplers demonstrate a higher affinity for polar to mid-polar compounds and much more work has been conducted with these types of samplers. In addition, for hydrophobic compounds, the more commonly used polymers appear to offer a more reliable quantification in single-phase applications. Polyethersulfone membranes are more often employed in dual-phase passive samplers: they are used in standard Polar Organic Chemical Integrative Samplers (POCIS), and often in Chemcatchers, as well as in organic Diffusive Gradients in Thin films (o-DGTs). Co-extracting the PES membranes of the dual-phase passive samplers along with the sorbent may help in better understanding the uptake kinetics to the receiving phases.

1. Introduction

Passive sampling of organic contaminants in water exploits the passive diffusion of chemicals from the aqueous phase to the receiving phase of the sampler [1]. This technique emerges among sample preparation techniques combining the sampling and the preconcentration steps directly in-situ and providing time-integrated water concentrations under specific conditions [2]. A passive sampler can be designed with a single phase or with two phases (Fig. 1).

The simplest design is the single-phase passive sampler, where the single polymeric sorption medium is directly exposed to the evaluated matrix [3,4]. Different polymers have been employed, such as polydimethylsiloxane (PDMS), polyoxymethylene (POM), Low Density Polyethylene (LDPE), etc. – generally for hydrophobic contaminants [4]. Some important differences between the various possible polymers exist, impacting their application in passive sampling. In several studies [5–9], polyethersulfone (PES), whose structure is shown in Fig. 2, was proposed for integrative passive sampling of less hydrophobic compounds, as an alternative to the more commonly used polymers.

Dual-phase passive samplers generally consist of a receiving phase covered by a protective membrane. The most diffused dual-phase passive samplers for polar compounds are POCIS, Chemcatchers and o-DGTs; these devices often use PES membranes, especially in the case of POCIS. In such applications, the membrane is increasingly being monitored for inducing lag times for mass transfer into the sorbent on the one hand, and as an important receiving phase for analyte accumulation on the other hand. In several POCIS studies, sampling rates (Rs) were even calculated for the protective PES membranes or for the whole device, due to substantial analyte uptake by PES.

The aim of this review is to summarize the information available in the literature on the use of PES as a receiving phase material in passive sampling, going from single-phase PES samplers to the peculiar contribution of PES in dual-phase samplers.

2. Polyethersulfone as a single-phase passive sampling material

2.1. An alternative material for less hydrophobic contaminants

Most publications on single-phase polymers as passive samplers have been on LDPE and PDMS samplers (also called silicon rubbers, SR), with a variety of studies on sampler performance and numerous field applications for neutral and relatively hydrophobic organic contaminants [4,10]. The use of SR in particular, has been growing due to the improved suitability for sampling, extraction and analysis, and faster

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* Corresponding author.
E-mail address: emanuele.magi@unige.it (E. Magi).

https://doi.org/10.1016/j.microc.2025.112958
Received 11 December 2024; Received in revised form 14 January 2025; Accepted 3 February 2025

polymer diffusion coefficients for hydrophobic organic contaminants in comparison with other applicable polymers [4,10]. LDPE passive samplers, on the other hand, are more efficient than SRs, due to easier procedures of precleaning before use and extraction [8]. However, both LDPE samplers and SRs have too low affinities for less hydrophobic and ionic contaminants. This results in less accumulation in the passive sampling devices and thus poorer detection possibilities. Thus, polymers more suited for moderately hydrophobic ($2 < \log K_{ow} < 5$) and ionic compounds, such as hormones, pharmaceuticals, and pesticides, are being investigated [11,12].

PES was first proposed by Prieto et al. as a sorptive material for microextraction of emerging pollutants from water samples because of its higher extraction yields for polar compounds in comparison with silicone rods and PDMS stir bars [13]. In the following years, PES has been used as free tubes for sorptive (micro)extraction of a wide variety of polar and non-polar chemicals (herbicides, pesticides, phthalates, hormones, personal care products, per- and polyfluoroalkyl substances (PFAS), benzotriazoles, corrosion inhibitors and alkylphenols) in environmental water samples at very low ng L^{-1} levels [14–20]. The extraction efficiencies of some of the less hydrophobic species by PES were significantly improved in comparison with other polymeric materials such as PDMS [14–20]. PES has also been employed for biological samples [21,22], with better uptakes than POM for the simultaneous extraction of alkylphenols, estrogens, bisphenol-A and a phthalate metabolite in fish biles [21].

Recently, PES has also been used in different formats (tubes/hollow fibres or flat-sheet membranes) as single-phase passive samplers for the study of compounds with a wide range of octanol – water partition coefficient ($\log K_{ow}$) in different water matrices. These include phthalates, PFAS, pharmaceuticals and personal care products (PPCPs), organochlorine pesticides, polychlorinated biphenyls, polycyclic aromatic hydrocarbons (PAHs) and UV filters [5–9]. Still, unlike for ex-situ applications, most of the compounds for which uptake was significant in situ are relatively non-polar.

2.2. Polyethersulfone membrane as a kinetic passive sampler

Accumulation of chemicals by passive samplers generally follows first order kinetics, which is characterized by an initial linear (kinetic/integrative) phase, followed by a curvilinear phase and a final equilibrium partitioning phase [23]. Passive samplers are employed in either kinetic or equilibrium sampling mode. In kinetic mode, the sampler remains in the linear uptake phase and the Time-Weighted Average (TWA) concentrations can be calculated for the whole deployment period using sampling rates [23]. Several studies have shown linear uptake for different classes of compounds using different PES samplers and are summarized in Table 1.

Posada-Ureta et al. compared Rs for musks, fragrances, organochlorine pesticides, phthalates and octylphenols for three different formats of PES samplers (free tube, PES tube enclosed in LDPE membrane, 0.1 μm-pore size PES flat-sheet membrane/filter) in a two-week calibration study [5]. In the comparison of the different configurations, higher Rs were observed for PES filters, due to the higher exposed surface area. The free PES tubes were also exposed in seawater to study 17 organic compounds, but were outperformed by SR due to the hydrophobicity of the studied analytes ($\log K_{ow}$ 4.30–8.62) [6]. Still, the performance strictly depends on the chosen analytes and deployment conditions. Using PES hollow fibres, 20 emerging contaminants (ECs) with a wide range of polarity were studied in another two-week calibration study in seawater [7]. While sampling rates could be calculated for 12 semi-polar compounds, these were much lower than in POCIS, and apparent equilibrium was reached after just 1 week. Scapuzzi et al. calculated 0.1 μm-pore size PES filter sampling rates for 4 UV filters and triclosan using 4-day exposures in tap water and synthetic seawater [9]. The performance of PES was compared with SR, showing higher polymer-water partition coefficients for PES, namely higher affinity for the polymer, for the compounds characterized by lower hydrophobicity but presenting specific chemical structures (aromatic rings and electron-withdrawing groups) [9]. Using 0.2 μm-pore size PES filters, an attempt was made by Chepchirchir et al. to model LogRs as a function of Abraham's descriptors using a linear solvation energy relationship (LSER) and 71 experimental Rs from 3 different studies [8]. However, the model resulted unsatisfactory ($R^2 = 0.63$) [8].

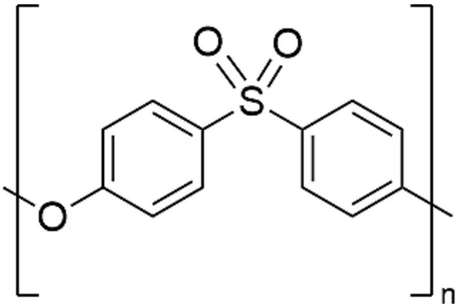

Fig. 2. Chemical structure of polyethersulfone.

Since sampling rates can be affected by environmental conditions [24], laboratory calibrations should be carried out to reproduce as reliably as possible field conditions. However, other options have been suggested, especially to account for water flow, which is one of the most impactful environmental factors affecting sampling rates in the case of water boundary layer-controlled uptake. Water flow can be measured in the field to better select lab-Rs [25,26]. Another solution is to use performance reference compounds (PRCs), which are '*analytically non-interfering substances*' that should follow the same R_s model as the target analytes [27]. PRCs have been successfully applied with several integrative hydrophobic passive samplers to correct for the influences of fouling and flow [4], while their use in polar passive samplers has been less successful so far [27]. Three studies have tested PRCs for PES single-phase passive samplers [5,7,8]. [$^2H_9$]-progesterone and [$^2H_5$]-atrazine displayed non-linear and low dissipation after 7 days of exposure [7].

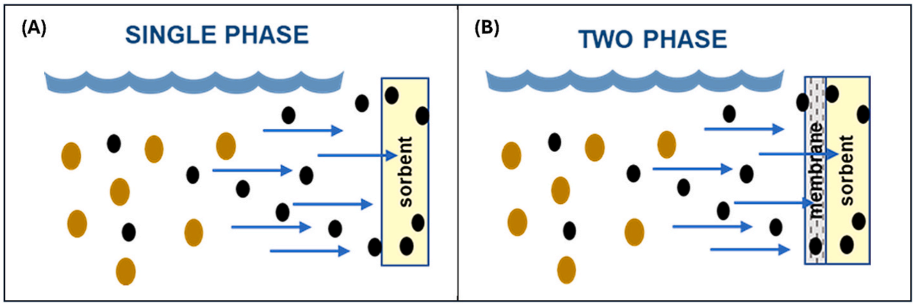

Fig. 1. Schematic representation of (A) single-phase and (B) two-phase passive samplers. The black circles represent the analytes in the aqueous matrix and the yellow circles other compounds present in the media.

Table 1
PES applications as a passive sampling medium in single-phase samplers.

Sampling configuration	Pore size/exposed surface area*	Analytes	Matrix	Recovery efficiency	Reference
Free PES tubes and flat-sheet membranes	0.1 μm/42 cm^2 (membranes), NR/52 mm^2 (tubes)	12 non-polar organic contaminants	WWTP effluents	NR	[5]
Free PES tubes	NR/52 mm^2	17 organic compounds	Seawater	NR	[6]
PES hollow fibers	NR/16 cm × 0.7 mm external diameter	20 ECs	Seawater	75–99 %	[7]
Flat-sheet membranes	0.2 μm/130 cm^2	31 PAHs, PCBs, and OCPs	River water	NR	[8]
Flat-sheet membranes	0.1 μm/90 cm^2	9 ECs	Marine waters	66–85 %	[9]

*As reported in the studies.
ECs: emerging contaminants, OCPs: organochlorine pesticides, NR: not reported, PAHs: polyaromatic hydrocarbons, PCBs: polychlorinated biphenyls, WWTP: wastewater treatment plant.

Several deuterated PAHs and PCBs have also been tested as potential PRCs but were also not applicable due to their nearly irreversible sorption to PES and poor curve fittings [5,8]. Considering PES membranes can uptake analytes through adsorption [9], finding adequate PRCs is not likely [27].

2.3. Polyethersulfone membrane in the equilibrium mode and K_{PESw} assessment

Differently from kinetic samplers, equilibrium sampling by single-phase passive samplers only requires the knowledge of polymer-water partition coefficients to estimate the aqueous concentration of a compound (C_w) [4]. In this case the accuracy of the calculated C_w of a particular compound strongly depends on the accuracy in the evaluation of its partition coefficient [28]. This parameter can be evaluated as the ratio of the concentrations of the analyte in the polymer and water phases once equilibrium in its partitioning has been achieved. Different methodologies can be used to estimate this coefficient, the most common being the constant C_w design (where the aqueous analyte concentration is kept constant) and the single dose design (an initial spike without further renewal) [28]. However, alternative methods could be used to avoid inaccurate measurements for the more apolar compounds due to the low aqueous phase concentrations, the possible sorption of chemicals to dissolved organic matter or to the container walls, and the very long equilibration times. The co-solvent method consists in the addition of an organic solvent to water in different proportions before extrapolating the pure water partition coefficient [28]. An aqueous boundary layer permeation method can also be employed: a preloaded PDMS disk serves as a donor phase while a pristine membrane piece serves as an acceptor phase [29]. A three-phase system has recently been proposed by adding a micelle-forming surfactant [30]. The polymer-water partition coefficient is calculated from the polymer-micelle partition coefficient in the three-phase system and the micelle water partition coefficient. Most of the studied compounds for sorption on PES are relatively polar; therefore, both the co-solvent method and the three-phase system may not be appropriate. Still, these other methods could be a welcome addition when using PES samplers for more hydrophobic classes – such as PAHs – that require a long time to reach equilibrium using the constant or single dose designs [8].

Experimental PES–water partition coefficient (K_{PESw}) values have been obtained using constant C_w or the single dose design for a variety of nonpolar and polar compounds either with a dual-phase device (POCIS and Chemcatcher) or with PES as a single-phase passive sampler. Table 2 summarizes a total of 13 different studies, including the LogK_{PESw} values obtained in a recent article which estimated K_{PESw} from graphical uptake data in the literature using image processing features [31].

Attempts to fit poly-parameter linear free energy relationships (PP-LFERs) with Abraham's descriptors to the K_{PESw} have been carried out in several works but the resulting fit was poorer for PES than for other homogeneous polymers such as PDMS or LDPE [8,31,35]. However, great care must be taken when examining the available data in the literature. Some of the reported K_{PESw} were estimated for compounds that were still in the integrative phase, and such values should not be considered to develop prediction models. In fact, out of the 13 studies directly reporting K_{PESw} values or from which K_{PESw} values were estimated, only five have verified "apparent" equilibrium, while full equilibrium attainment was not verified for the others (Table 2). In addition, compound recovery from PES through the selected extraction procedure is not always verified, making the estimation even more uncertain. Thus, accurate PES-water partition coefficients remain poorly documented in the literature. Furthermore, competitive sorption has also been suggested to have potential influence on the sorption [41]. Better quality data is certainly required to improve models. All K_{PESw} values for which partial equilibrium has been reportedly verified are reported in Table 3.

Table 2
Summary on the information regarding LogK_{PESw} assessment studies.

Study	Number of compounds	Exposure type	Compound recovery assessment	Partial equilibrium verified
[32]	26	Single (flat-sheet)	Not reported	Yes
[13]	16	Single (tube)	Not reported	No
[33]	14[a]	Dual (POCIS and Chemcatcher)	Not reported	No
[31] (using data from [34])[b]	8	Dual (POCIS)	Not reported	No
[35]	14	Single (flat-sheet)	Yes	Yes
[36]	29	Dual (POCIS)	Not reported	Yes
[37]	33	Dual (POCIS)	Not reported	For the whole POCIS
[38]	8	Dual (POCIS and Chemcatcher)	Yes	No
[39]	18	Dual (POCIS)	Yes	No
[40]	12	Single (flat-sheet)	Yes	No
[8]	30	Single (flat-sheet)	Not reported	No
[31]	4	Single (flat-sheet)	Yes	Yes
[9]	9	Single (flat-sheet)	Yes	Yes

[a] Up to four K_{PESw} values per analyte (four different Chemcatcher or POCIS configurations). [b] Suchana et al. extracted graphical uptake data from Silvani et al. (2017) using image processing features to estimate K_{PESw} values.

It must be pointed out that PES has not been used as an equilibrium passive sampler (except in one study using POCIS [37]). Furthermore, some authors have suggested that the time required to reach true equilibrium for PES-water partition may be too long for use of PES as an equilibrium passive sampler [31]. On the other hand, K_{PESw} values are of great value to improve understanding of the uptake of polar chemicals of interest by dual-phase passive samplers and model their performance [23,31,42]. K_{PESw} may also allow to exclude from attempting to apply dual-phase passive samplers to analytes which tend to sorb to the PES membrane [31].

Table 3
Individual LogK$_{PESw}$ values (L/kg) for which partial equilibrium has been verified.

LogK$_{PESw}$ < 3		$3 <$ LogK$_{PESw}$ < 4		LogK$_{PESw}$ > 4	
Compound	LogK$_{PESw}$	Compound	LogK$_{PESw}$	Compound	LogK$_{PESw}$
Acebutolol	1.48 [36]	Acetanilide	3.49 [35]	Benzophenone-3	4.52 [9]
Acetochlore	2.72 [36]	Atrazine	2.84 [36], 3.68 [32]	1-cyanonaphthalene	5.48 [35]
Benzotriazole	2.84 [32]	Benzimidazole	3.38 [35]	Diazinon	4.50 [32]
Betaxolol	2.86 [36]	Bisphenol A	2.56 [9], 3.38 [36]	3,4-dichloroaniline	3.86 [31], 4.81 [36]
Bezafibrate	1.90 [36]	Caffeine	2.52 [32], 3.13 [35]	Diuron	4.01 [36], 5.04 [32]
Bisoprolol	2.00 [36]	Carbendazim	3.16 [36], 3.76 [32]	Ethyl hexyl methoxy cinnamate	4.25 [9]
Carbamazepine	2.40 [36], 2.90 [32]	Chloridazon	3.50 [32]	Indole	4.57 [35]
Diclofenac	2.54 [36], 2.60 [32]	4-chloronitrobenzene	3.44 [31]	Isoproturon	4.20 [32]
2,4-dichlorophenoxyacetic acid	1.30 [36]	Deisopropylatrazine	3.18 [32]	Linuron	4.21 [36]
Estrone	2.62 [9]	Desethylatrazine	3.37 [32]	2-methoxynaphthalene	5.73 [35]
17α-ethinyl estradiol	2.62 [9]	3,4-dichloronitrobenzene	3.60 [31]	4-methylbenzylidene camphor	4.26 [36]
Furosemide	2.04 [36]	2,4-dichlorophenol-d3	3.33 [36]	1-naphthaleneacetamide	4.46 [35]
Hydroxyatrazine	1.58 [32]	Estriol	3.04 [36]	4-nitroaniline	4.23 [35]
Ketoprofen	1.90 [36]	Irgarol	3.90 [32]	Octocrylene	4.58 [9]
Mecoprop	1.07 [32]	Megestrol	3.60 [36]	Octyl dimethyl p-aminobenzoate	4.35 [9]
Metoprolol	1.90 [36]	5-methylbenzotriazole	3.42 [32]	Triclosan	4.13 [9]
Naproxen	1.95 [36]	Metolachlor	3.13 [32]		
Oxprenolol	1.85 [36]	2-nitrotoluene	3.38 [31]		
Phenazone	2.38 [32]	Phenol	3.16 [35]		
Sufamethoxazole	2.49 [32]	Prochloraz	3.93 [36]		
Sulcotrione	0.72 [32]	Progesterone	3.52 [36]		
Testosterone	2.48 [36]	Terbuthylazine	3.67 [32]		
Timolol	1.30 [36]	Terbutryn	3.91 [32]		
Trimethoprim	1.78 [36]	Umbelliferone	3.96 [35]		
		β-estradiol	2.22 [9], 3.08 [36]		

3. PES membrane as a potential passive sampling material in dual-phase samplers

3.1. Sorption to the membrane and its impact on sorbent uptake

A diffusive membrane is generally employed in dual-phase passive sampling to protect the sorbent and lengthen the linear uptake phase. Chemicals first diffuse through water to the membrane where they may be sorbed. Then, they diffuse through the membrane to the sorbent where they accumulate. Since the first evidence of analyte sorption into PES membranes [43], growing attention has been paid to the possible presence of lag times in the uptake into the sorbent of dual-phase samplers and to the potential use of the membrane itself as receiving phase.

A total of 30 studies have co-extracted the PES membranes from exposed dual-phase samplers. In 20 of these publications, PES membranes were co-extracted from dual-phase samplers in laboratory studies [31,32,34,36–40,42,44–54]. In 14 papers, PES membranes were co-extracted from dual-phase samplers as a sampling strategy in field studies [5,37,39,43,51,52,55–62]. Overall, most of the studies regarding PES uptake of contaminants in dual-phase applications have been for POCIS applications, where generally PES is the default membrane. It is possible that better alternative membranes could be used in the future for POCIS [63]. Nevertheless, considering the extent of the use of standard POCIS, which are already accepted in some regulatory monitoring [64], PES membranes will continue being used in the foreseeable future. Hence, it is fundamental to understand the role of PES in dual-phase samplers. An increasing number of studies have extracted PES membranes [32,36,39,45,53,59,62] in addition to the internal sorbent, and in many, large fractions of certain contaminants were measured on the standard PES membrane in respect to the whole POCIS. This was especially observed in the first hours of deployment, followed by diffusion towards the sorbent, thus representing a lag phase in the contaminants' uptake to the inner phase. Compounds with logK$_{PESw}$ ≥ 4 were found to primarily accumulate on POCIS membranes (PES) during typical deployment durations [40]. So in these cases, when the lag phase is important compared to the total sampler deployment time, the conventional TWA estimation may be less accurate, since connected to an "immediate" analyte accumulation to the sorbent [32]. Another recent example dealing with the distribution of specific compounds between the PES and hydrophilic-lipophilic balance (HLB) phases combined POCIS sampling with compound-specific stable isotope analysis (CSIA) for substituted chlorobenzenes. In that study, a higher accumulation of heavier isotopes in the POCIS was concluded to be due to PES accumulation, highlighting once again its important role in these dual-phase passive samplers [55]. Using PES membranes with larger pores may help in dealing with this issue, since by reducing the pore surface area within the membrane matrix, the partitioning between the PES and the sorbent phases is shifted towards the sorbent [45,63].

To estimate the impact of the membrane on the sorption into the receiving phase, Kaserzon et al. proposed to assess the limiting step of the uptake by the relationship between the sampling rate and the polymer-water partition coefficient. A positive linear correlation between these two parameters implies the transport is under membrane control [54]. Indeed, the sampling rate is proportional to the overall mass transfer coefficient which depends on the mass transfer coefficients of the involved compartments (e.g., WBL, membrane and sorbent) and the partition coefficients between them. However, the application of this method is limited to the transport via the polymer phase and not via water-filled pores [54]. In fact, if the transport through the membrane is controlled by the diffusion in the pore water, it should be independent of the partition coefficient but dependent on the water diffusion coefficient related to the molecular size of the analyte.

Analyte sorption to the PES membranes was also assessed in several Chemcatcher calibration studies to improve understanding of uptake kinetics and possible lag phases to the sorbent disk [32,44,47–49]. In two such studies, no substantial sorption took place, so analysis of the PES membrane was later forsaken [47,48]. On the other hand, Becker et al. observed some minor lag times for the uptake of several compounds using styrene–divinylbenzene reversed phase sulfonated polymers (SDB-RPS), due to sorption to the 0.2 μm-pore size PES protective membranes [49]. Vermeirssen et al. observed that using Chemcatchers with SDB disks and 0.1 μm-pore size PES protective membranes, lag phases could occur for analytes with logK$_{PESw}$ > 2 [32]. On the other hand, Glanzmann et al. observed no significant lag phases, even if there was considerable sorption by PES for most of the studied compounds [44]. In a study on glass fibre filter- Envi-Carb "sandwich" disks, the sorption of the analytes onto the PES membranes were assessed and substantial accumulation of a herbicide was observed; despite this, uptake to the sorbent disk was linear, so the authors decided to no longer extract the membrane [46].

3.2. Single membrane sorption assessments prior to membrane selection in dual-phase samplers

From the considerations above, it appears clear that strategies to avoid or to deal with the sorption of target chemicals in the protective membrane are necessary. In general, the basic rule is that this membrane should retain as little of the target chemicals as possible so as to not complicate the accumulation process; ideally, only diffusion into the pore water should take place. During sampler configuration development, it is thus recommended to check for potential sorption to the membrane for different organic chemical classes.

PES sorption was verified prior to selecting the right membrane in several recently developed passive samplers: for PASSIL applications (passive sampling using ionic liquids as the receiving phase) [65,66] and for an equilibrium sampler using ultra-pure water as a receiving phase for PFAS [67].

Using a mechanistically based, one-dimensional diffusion model, Endo et al. recommended that $\log K_{PESw}$ should be <3 or <4 (see Table 3 for examples of compounds with such values) in the standard Chemcatcher setting to avoid a lag time of >1h or >1 d in the sorbent disk respectively [68]. If such compounds are to be studied, an alternative membrane or no membrane at all are possible alternatives.

In several o-DGT studies, potential analyte sorption was preliminarily assessed for different membrane materials including 0.45-μm pore size PES membrane filter disks to evaluate their possible use in o-DGT configurations. These sorption experiments were usually conducted for 4–24h in a small volume of water (5–25 mL) spiked with a high initial concentration of analyte (typically 100 $\mu g\ L^{-1}$, in the range 10 $\mu g\ L^{-1}$ – 1 $mg\ L^{-1}$) [64,69–86]. Concentrations of the analytes before and after the exposure were measured in the water to evaluate the possible adsorption to the PES membrane. In most cases, sorption was reported as adsorption efficiencies defined as the analyte fraction adsorbed (the ratio between mass of analytes in the single membrane and total mass in the initial solution in %) and as the mass adsorbed (μg) per filter membrane area [87]. Some of these results are summarized by Ji et al. [87], who plotted the fraction adsorbed (%) of tested organic compounds by the PES membrane used in the o-DGT devices versus $\log K_{ow}$ values of tested analytes. High fractions adsorbed were shown for some hydrophilic compounds with $\log K_{ow} <3$; of particular note, fractions >28% for second-generation fluoroquinolones with $\log K_{ow} <0$ (norfloxacin, ofloxacin, pefloxacin, ciprofloxacin, enrofloxacin) and close to 100% for methylparaben ($\log K_{ow} = 1.67$) were reported. The number and mass of compounds accumulated onto the PES membranes decrease with increasing PES membrane pore size [64].

In two POCIS studies, PES membrane controls, i.e., POCIS without the sorbent, were also exposed to target compounds. PES membrane controls were compared to POCIS after 10 d of exposure to water spiked with the analytes: the ratio of the mass of the target compound in the PES membrane (controls) and the mass of the target compound retained by the sorbent (POCIS device) was lower than 0.1 for all tested compounds, which meant that the target compounds did not greatly accumulate in the PES membrane and could quickly transfer to the sorbent [88]. In another study, PES membrane controls were also tested for two pesticides, for 7 d. A substantial amount of pesticide was retained by the PES membranes and may affect the uptake by the POCIS sorbent [89].

Even though these evaluations are essential in better understanding the distribution of the analytes in dual-phase samplers, it is important to bear in mind that these systems are more complex than single membranes. Indeed, unlike for single PES membranes, the accumulation of the analytes in PES from dual-phase samplers may be lower due to internal mass redistribution from the PES to the sorbent [31].

3.3. Dealing with PES membrane sorption by co-extracting PES membranes

Field applications where PES membranes in dual-phase samplers were extracted as a sampling strategy are listed in Table 4 and discussed throughout this section.

3.3.1. Separate extraction and separate assessment

In an important laboratory study, Vermeirssen et al. assessed and modelled the transfer of polar compounds over PES membranes in Chemcatchers and POCIS [32]. A three-compartment first order kinetic model was introduced for the uptake by the sorbent in Chemcatchers and POCIS of 22 compounds of various classes (herbicides, pharmaceuticals and industrial chemicals). Compared to the traditional sampling rate model, the multi-compartment model better fitted the data for compounds that strongly sorb to the PES membrane leading to lag phases [32]. However, in extreme cases, when the analyte concentration is very low in one compartment (either sorbent or PES membrane), the estimation of K_{PESw} could be affected by large errors. Thus, the model should be simplified by excluding the compartment where the concentration is very low compared to the other compartment. Estoppey et al., used a simplified two-compartment model for POCIS and Chemcatchers by excluding the sorbent compartment for six nitroaromatic compounds ($1.54 < \log K_{ow} < 2.37$) which mainly partitioned to the PES membrane but not to the sorbent [39]. In further field deployments in lake-bottom waters, these six nitroaromatics were therefore extracted solely from the PES membranes.

Two recent studies have assessed the potential benefit of co-extracting PES membranes alongside o-DGT or POCIS sorbents on a larger scale. Castro et al. used four chromatographic separation modes for the suspect screening of 3227 chemicals (pharmaceuticals, pesticides, drugs of abuse, human metabolites, industrial chemicals among others) in surface waters by analysing 0.45-μm pore size POCIS PES membranes and sorbent extracts [60]. The number of compounds identified in the POCIS membrane (23 compounds) was much lower than the number of compounds detectable in the POCIS sorbent (115 compounds). This led to the decision not to analyse the membrane extract as a sampling strategy. This may be on account of the type of contaminants in the suspect screening library, as only 25% of the investigated chemicals can be considered as nonpolar, namely characterized by an octanol–water distribution coefficient > 3.2 at neutral pH ($\log D_{pH\ 7} > 3.2$) [90,91]. Indeed, the logD of the compounds found in the POCIS membrane was statistically higher than the logD of those found in the POCIS sorbent extracts [60]. In addition, the PES membranes used were of a greater pore size than commercial POCIS (0.45 vs 0.1 μm), which tends to shift the partitioning towards the sorbent [45]. While assessing the applicability of o-DGTs and POCIS to collect a wide range of analytes, Renaud et al. also extracted the PES membranes separately from both types of devices and screened them for 299 target compounds [61]. They concluded that only a small benefit arises from extracting the membrane of the o-DGT devices, as few additional compounds were detected exclusively on the PES membranes. In contrast, for POCIS, extracting 0.1-μm pore size PES membranes alongside the HLB sorbent resulted advantageous to increase the number of compounds detected. However, the targeted analytes were relatively polar: most had ($\log D_{pH\ 7} < 3$), which greatly limits the assessment of the potential benefit of co-extracting PES membranes to polar and semipolar compounds only.

Jeong et al. calculated water equilibrium concentrations from PES extracts for 21 compounds in a wastewater treatment plant effluent and river waters after 35-d deployments of POCIS. These equilibrium concentrations were compared to TWA concentrations from the POCIS sorbent. For most compounds, the calculated concentrations by both methods were similar or at least in the same range, while for several compounds, the concentrations calculated by both methods were very different [37]. Analyte recovery was not reported in the study. However,

Table 4
PES field applications as a passive sampling medium in dual-phase samplers.

Sampling configuration	Application strategy	Pore size/surface area*	Analytes	Matrix	Recovery efficiency	Reference
PES tubes enclosed in LDPE membranes	A	NR/52 mm^2	12 non-polar organic contaminants	WWTP effluents	NR	[5]
POCIS-like sampler flat-sheet membranes	B	0.45 µm/16 cm^2	9 PFAS	River water	NR	[52]
POCIS flat-sheet membranes	B	0.1 µm/NR	23 polar pesticides and 8 metabolites	River water	NR	[59]
POCIS flat-sheet membranes	B	0.1 µm/90 mm diameter	34 pesticides and pharmaceuticals	Deionized water	NR	[37]
Chemcatcher and POCIS flat-sheet membranes	B	0.1 µm/90 and 47 mm diameters respectively	18 nitroaromatic compounds	Lake-bottom waters	49–96 % and 24–64 %, respectively	[39]
POCIS flat-sheet membranes	B	0.1 µm/45.8 cm^2	37 target compounds	River water and WWTP effluent	NR	[51]
POCIS flat-sheet membranes	B	0.45 µm/47 mm diameter	Suspect screening of 3227 chemicals	Wastewater and surface water	NR	[60]
POCIS and o-DGT flat-sheet membranes	B	0.1 µm/41 cm^2 exposed (POCIS) NR/3.1 cm^2 exposed (o-DGT)	299 target analytes	Surface water	NR	[61]
POCIS flat-sheet membranes	B	0.1 µm/45.8 cm^2 exposed	9 ECs	Wastewater effluent	From [9]	[62]
POCIS flat-sheet membranes	B	0.1 µm/≈40 cm^2	6 substituted benzene compounds	Wetland fed by partially treated groundwater from an industrial site	74–85 %	[55]
Chemcatcher flat-sheet membrane	C	0.2 µm/47 mm diameter	9 herbicides	Drinking water	Additional extraction with the same procedure to verify no further release of analytes	[43]
POCIS flat-sheet membranes	D	0.1 µm/90 mm diameter	319 pesticides	Alpine streams	Calculated for the whole POCIS	[56]
POCIS-like samplers flat-sheet membranes	D	0.22 µm/10 cm^2	50 ECs	River and lagoon waters	NR	[58]
POCIS-like samplers flat-sheet membranes	D	0.1 µm/41 cm^2	7 ECs	WWTP influent and its receiving water	NR	[57]

* As reported in the studies.
A: extraction of the PES material only, B: separate extraction and separate assessment, C: separate extraction and combined uptake assessment, D: combined extraction and combined uptake assessment.

by using ultra-pure water to recover the sorbent from the POCIS, some of the polar analytes may have been lost from either or both compartments leading to such differences. A sudden increase or decrease in water concentration in the few days prior to the end of the deployment may also have led to a higher or a lower equilibrium concentration in the PES respectively compared to the average concentration for the whole period measured by the HLB sorbent. Thus, while comparing estimated water concentrations from different samplers is always informative, using the PES to estimate the concentrations of polar compounds with poor affinity for the membrane is certainly not feasible.

3.3.2. *Separate extraction and combined uptake assessment*

Tran et al. extracted both the PES membranes (0.2 µm) and the sorbent disks of Chemcatchers separately to study the partition between the two compartments. Due to the higher accumulation of diuron in the membrane, the authors decided to calculate sampling rates of the studied herbicides based on the accumulated amounts of the analytes on the whole device. They concluded that these sampling rates could be used to calculate TWA concentrations from the accumulated amount of the analytes by the whole device in field studies [43].

In a laboratory study, Silvani et al. investigated the uptake of alkylphenols by both compartments of POCIS. Both sorption to the PES and to the HLB were linear. As alkylphenols with high hydrophobicity ($\log K_{ow} \geq 4$) were primarily accumulated in the PES membranes, for each analyte the amounts adsorbed onto both Oasis HLB and PES were summed to calculate “combined” POCIS sampling rates. This approach was strongly advocated to monitor the concentration of these chemicals more effectively in water by allowing the accumulation of hydrophobic as well as hydrophilic alkylphenols using just one passive sampler [34].

In another laboratory study, Djomte et al. also extracted PES and HLB from POCIS separately, and assessed the sampling rates of both phases singly and combined, to assess the potential improvement in sampling rate estimations. For 4 compounds with $\log K_{PESw} \geq 3.9$, a large portion partitioned to the PES membrane (47 to 96%) and sorption to the PES and to the HLB were both linear. Thus, Rs calculated with mass adsorbed to HLB plus PES membranes would improve the sensitivity related to sampling rate estimations for these compounds. However the meaningful gains in sensitivity may be offset by an increased susceptibility to changing environmental conditions (exposure to water with added sediment led to reduced accumulation on the PES in their study thus reducing the combined sampling rates) [40].

Suchana et al. extracted the PES and sorbent phases in POCIS separately [55]. Both phases were significant sinks for the target compounds. When combining the PES and sorbent extracts, the minimum water concentration required for precise and accurate C-, H- and N-CSIA of the target compounds was improved. Combining multiple PES or PES and HLB extracts also improved the detection limits.

3.3.3. *Combined extraction (and combined assessment)*

Recently (2023–2024), the PES membranes and the sorbents from dual-phase passive samplers have been combined for assessment of the uptake by the whole samplers. The sorbent and the PES membranes of POCIS were extracted together in a study on pesticides in alpine streams. In situ sampling rates of the total POCIS were calculated for 31 pesticides with a wide range of polarity, and field validation showed that most of these Rs were robust for different sampling periods and sampling sites [56]. Six pharmaceuticals and one artificial sweetener were also extracted from whole POCIS deployed in rural headwater streams upstream and downstream from on-site wastewater disposal systems, and in-situ Rs were also calculated [57]. Considering the low hydrophobicity of the studied compounds, these 'whole POCIS' Rs are expected to be equivalent to the Rs if only the sorbent had been extracted. In a study regarding metal–organic frameworks in passive sampling devices (MOFs-PSDs, i.e., POCIS-like samplers), the sorbent and the PES membranes were also extracted together for a wide group of ECs ($\mathrm{LogD_{pH\ 7}}$ from −5.0 to 5.0). Some of the compounds (including the more hydrophobic ECs), were successfully calibrated to yield lab-Rs [58].

While only these three cited studies have co-extracted both the PES membranes and the sorbents from dual-phase passive samplers, partial co-extraction may have taken place in other studies that focused on the sorbent only. In several POCIS studies, methanol was used to transfer the solid phase from the PES membranes to an SPE column for extraction, and this wash solution was usually combined to the eluate [92–100]. Ionic liquids were also recovered from the PES membranes of PASSIL samplers using a large volume of acetonitrile [101]; while the PES membranes from Chemcatchers were rinsed with acetone, the eluate then used to also extract the Chemcatcher sorbent disk in a study on triazines [102]. Thus, the authors may have already partially co-extracted the PES membrane for compounds which can sorb onto it. When sampling rates from the literature related to the single sorbent compartment extraction were used to estimate TWA concentrations, the total Rs may have been underestimated leading to an overestimation of the TWA concentrations [98,99,103].

Furthermore, in the study of Challis et al., important signal suppression in the negative mode impacted the analysis of several compounds and was assumed to be due to matrix effects from the membrane co-extraction, especially as the membrane had not been pre-washed [99]. This was corroborated by Jeong et al. who measured the ionization effects in the electrospray ionization (ESI) source during the LC–MS/MS analysis of Oasis HLB sorbent and PES membrane extracts, finding more variable ionisation factors for the PES extracts, likely due to biofouling [37]. Indeed, organic matter adhering on the membranes can be difficult to remove. In contrast, the sorbent is not directly exposed to the environment and is thus more protected from biofilm growth. If the membrane is heavily fouled, the resulting matrix effect could lead to an excessive decrease in sensitivity when pooled sorbent-membrane extracts are analysed, especially for compounds that tend to partition to the sorbent rather than the membrane. This implies that PES membranes and the sorbent should be extracted and analysed separately for more accurate results [51]. In addition, combined uptake kinetics may be more complex to understand than by extracting both compartments separately. This is compounded by the lack of information on the recovery efficiencies during extraction of analytes accumulated on the membranes [63], as well as the lack of information on stability during membrane storage before analysis [104]. However, Casari et al. demonstrated that in situ sampling rates of pesticides from total POCIS extraction (HLB sorbent + PES membrane) applied to different alpine streams well agreed with spot sampling values [56]. Compared to the study by Jeong et al., this was conducted for a shorter period of time (21 vs 35 days) and in more "pristine" rivers with less and more easily removable fouling appearing on the membranes.

4. Future perspectives on the use of PES as a receiving phase in passive sampling

Compared to other single-phase passive samplers, not much work has been carried out with PES as a single-phase passive sampler. For the more hydrophobic compounds, several single-phase passive samplers such as SR and LDPE are better understood and more robust, as PRCs offer a good correction of the impact of water flow. On the other hand, adsorption is the main mechanism of sorption onto PES, thus, more complex kinetics are involved compared to the simpler absorption in SR and LDPE. Furthermore, due to this complexity, PRCs are not suitable for correcting the impact of water flow on PES samplers. In addition, PES is not used as an equilibrium passive sampler, due to the long equilibrium times required for hydrophobic compounds. For more polar compounds, the already existing traditional dual-phase polar samplers (POCIS, Chemcatcher, o-DGT) are not only better characterized than PES samplers [105,106], but the receiving phase in these samplers has a much higher affinity for more polar compounds than PES. Overall, the polyethersulfone membrane as a single-phase passive sampler may be less competitive compared to other types of passive samplers and thus may not fuel further research in that field.

While many studies have measured dual-phase passive sampler sorbent sampling rates for a large range of polar compounds using calibration studies, very few have measured the protective membrane partitioning coefficient. Nonetheless, measurements of the polymer–-water partition coefficients are needed to improve understanding of the uptake of polar chemicals of interest by dual-phase passive samplers with PES membranes and model their performance. A decision tree may be useful to select the best approach to follow (Fig. 3).

In dual-phase passive sampler applications, the membrane should be co-extracted if compounds likely to be affected by lag-phases are part of the study. As described in depth above, different extraction and Rs assessment strategies can be employed to take into account the sorption both in the sorbent and in the PES membrane. If the analyte accumulates mainly in one compartment of the sampler and uptake is integrative, the extraction of the single compartment is suggested, and the related sampling rate should be used to estimate the analyte concentration in the studied environment. Indeed, if the amount of the analyte in the PES is negligible compared to the amount accumulated in the sorbent, the overall sampling rate (sorbent and PES) corresponds to the Rs of the sorbent. This occurs for most polar and semi-polar compounds over typical deployment durations. On the contrary, for the more hydrophobic compounds the uptake mainly occurs in the PES membrane. In this scenario, the sampling rate in PES can be used to determine the TWA concentration ($\mathrm{Rs}_{\mathrm{hydrophobic}}$ (sorbent+PES) ≈ $\mathrm{Rs}_{\mathrm{hydrophobic}}$ PES). For compounds that partition to both the PES and the sorbent, more work is needed to assess if the combined Rs can reduce the issues related to internal mass redistribution (e.g. lag phase for the sorbent) that is affected by field conditions. In fact, the mass redistribution is linked to the mass transfer resistances involved in sorption which in turn are related to the thickness of the phases present and the partition coefficients. For instance, the presence and the nature of fouling/sediment can reduce the transport across the protective layer (limiting the interactions with the membrane surface or blocking the pores) or enhance the sorption in the whole sampler adding a new phase with different affinity for the target compounds. Considering the latter scenario, an additional mass transfer resistance must be considered. This affects the sorbent Rs since it is dependent on the overall mass transfer resistance [107,108]. As a consequence, the accuracy in the evaluation of the TWA concentration is influenced by the presence and the nature of the new layer.

Combined extraction would reduce time and cost of the analysis compared to separate extraction. However, this improvement may be offset by an increased susceptibility to changing environmental conditions and the different extraction efficiencies of the two receiving phases. Thus, an important factor in the decision to extract or not the membrane may be the deployment time. For long exposures in complex matrices (marine waters, wastewaters) leading to heavy biofouling of the membranes, it may not be feasible or recommended to co-extract the membrane due to increased signal suppression. In addition, results from controlled laboratory experiments may not be easily applied to complex field applications where substantial (bio)fouling has taken place altering the membrane sorption kinetics. On the other hand, for shorter deployment times in relatively clean freshwater matrices (mountain rivers, drinking water), combined extraction appears feasible and could be advantageous.

5. Conclusion

In this review, an insight into the possible use of polyethersulfone

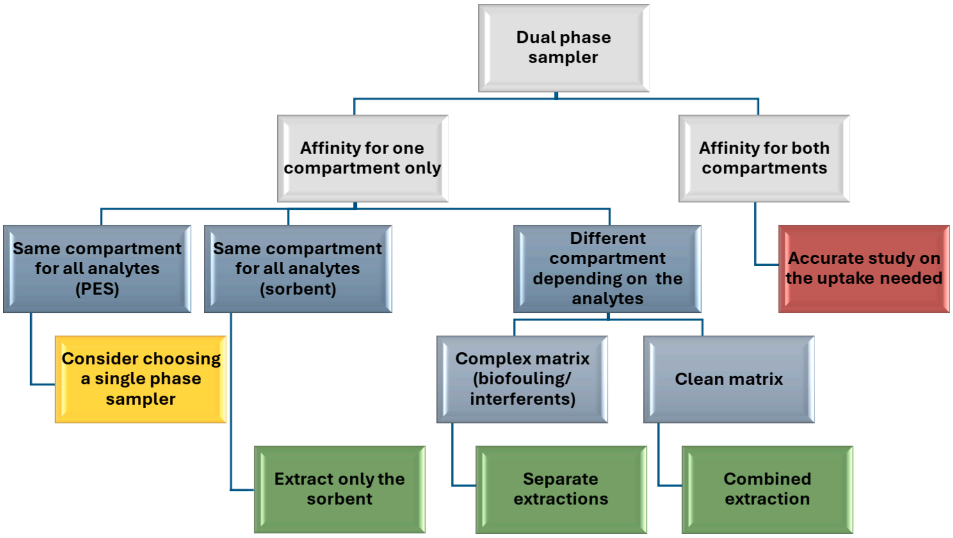

Fig. 3. Decision-tree to select the best approach when dealing with dual-phase passive samplers and extraction of analytes with different affinities for the compartments.

membranes as passive samplers was given. In the form of a single-phase sampler, PES appears not to be competitive enough compared to other types of samplers, thus maybe discouraging further developments. On the other hand, assessing uptake of analytes by PES in dual-phase samplers may be useful, or even required. Most of the studies regarding PES uptake of contaminants have indeed been for dual-phase passive samplers, especially POCIS. For these devices, co-extracting PES membranes alongside sorbents may allow not only to increase the number of more hydrophobic compounds detected, but also to improve understanding of the uptake of polar/mid-polar chemicals by dual-phase passive samplers, thus better modelling their performance. Combining the extracts during sample processing may lead to meaningful gains in sensitivity in pristine environments. Still, an increased susceptibility to ion suppression in more complex matrices could be observed, suggesting a careful evaluation of the procedure to employ in different situations.

CRediT authorship contribution statement

Henry MacKeown: Writing – review & editing, Writing – original draft, Investigation, Formal analysis, Data curation, Conceptualization. **Chiara Scapuzzi:** Writing – original draft, Investigation, Data curation. **Barbara Benedetti:** Writing – review & editing, Visualization, Validation. **Marina Di Carro:** Writing – review & editing. **Emanuele Magi:** Writing – review & editing.

Funding

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

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.

Data availability

Data will be made available on request.

References

[1] S. Seethapathy, T. Górecki, X. Li, Passive sampling in environmental analysis, J. Chromatogr. A 1184 (2008) 234–253, https://doi.org/10.1016/j.chroma.2007.07.070.

[2] D.A. Alvarez, J.D. Petty, J.N. Huckins, T.L. Jones-Lepp, D.T. Getting, J. P. Goddard, S.E. Manahan, Development of a passive, in situ, integrative sampler for hydrophilic organic contaminants in aquatic environments, Environ. Toxicol. Chem. 23 (2004) 1640–1648, https://doi.org/10.1897/03-603.

[3] F. Salim, T. Górecki, Theory and modelling approaches to passive sampling, Environ. Sci. Process. Impacts. 21 (2019) 1618–1641, https://doi.org/10.1039/c9em00215d.

[4] A.C. Taylor, G.R. Fones, B. Vrana, G.A. Mills, Applications for Passive Sampling of Hydrophobic Organic Contaminants in Water—A Review, Crit. Rev. Anal. Chem. 51 (2021) 20–54, https://doi.org/10.1080/10408347.2019.1675043.

[5] O. Posada-Ureta, M. Olivares, L. Zatón, A. Delgado, A. Prieto, A. Vallejo, A. Paschke, N. Etxebarria, Uptake calibration of polymer-based passive samplers for monitoring priority and emerging organic non-polar pollutants in WWTP effluents, Anal. Bioanal. Chem. 408 (2016) 3165–3175, https://doi.org/10.1007/s00216-016-9381-7.

[6] O. Posada-Ureta, M. Olivares, A. Delgado, A. Prieto, A. Vallejo, M. Irazola, A. Paschke, N. Etxebarria, Applicability of polydimethylsiloxane (PDMS) and polyethersulfone (PES) as passive samplers of more hydrophobic organic compounds in intertidal estuarine environments, Sci. Total Environ. 578 (2017) 392–398, https://doi.org/10.1016/j.scitotenv.2016.10.194.

[7] L. Mijangos, H. Ziarrusta, A. Prieto, O. Zugazua, O. Zuloaga, M. Olivares, A. Usobiaga, A. Paschke, N. Etxebarria, Evaluation of polar organic chemical integrative and hollow fibre samplers for the determination of a wide variety of organic polar compounds in seawater, Talanta 185 (2018) 469–476, https://doi.org/10.1016/j.talanta.2018.03.103.

[8] B.S. Chepchirchir, X. Zhou, A. Paschke, G. Schüürmann, Polyethersulfone as suitable passive sampler for waterborne hydrophobic organic compounds – Laboratory calibration and field test in the Sosiani river, Kenya, Sci. Total Environ. 699 (2020) 134056, https://doi.org/10.1016/j.scitotenv.2019.134056.

[9] C. Scapuzzi, H. Mackeown, B. Benedetti, M. Baglietto, M. Di Carro, E. Magi, Polyethersulfone membrane as a single-phase passive sampler : Evaluation of the sampling performance for emerging contaminants in water, Microchem. J. 195 (2023) 109445, https://doi.org/10.1016/j.microc.2023.109445.

[10] J. Sobotka, F. Smedes, B. Vrana, Performance comparison of silicone and low-density polyethylene as passive samplers in a global monitoring network for aquatic organic contaminants, Environ. Pollut. 302 (2022) 119050, https://doi.org/10.1016/j.envpol.2022.119050.

[11] K.E.C. Smith, Passive Sampling for Determination of the Dissolved Concentrations and Chemical Activities of Organic Contaminants in Soil and Sediment Pore Waters, Handb, Environ. Chem. 100 (2020) 351–368, https://doi.org/10.1007/698_2020_572.

[12] W. Lao, Y. Hong, D. Tsukada, K.A. Maruya, J. Gan, A new film-based passive sampler for moderately hydrophobic organic compounds, Environ. Sci. Technol. 50 (2016) 13470–13476, https://doi.org/10.1021/acs.est.6b04750.

[13] A. Prieto, R. Rodil, J.B. Quintana, I. Rodríguez, R. Cela, M. Möder, Evaluation of low-cost disposable polymeric materials for sorptive extraction of organic pollutants in water samples, Anal. Chim. Acta. 716 (2012) 119–127, https://doi.org/10.1016/j.aca.2011.12.023.

[14] J. Casado, I. Rodríguez, M. Ramil, R. Cela, Polyethersulfone solid-phase microextraction followed by liquid chromatography quadrupole time-of-flight

mass spectrometry for benzotriazoles determination in water samples, J. Chromatogr. A 1299 (2013) 40–47, https://doi.org/10.1016/j.chroma.2013.05.061.

[15] L. Blanco-Zubiaguirre, A. Delgado, O. Ros, O. Posada-Ureta, A. Vallejo, A. Prieto, M. Olivares, N. Etxebarria, Assessment of commercially available polymeric materials for sorptive microextraction of priority and emerging nonpolar organic pollutants in environmental water samples, Environ. Sci. Pollut. Res. 21 (2014) 11867–11883, https://doi.org/10.1007/s11356-013-2481-4.

[16] J. Cavalheiro, M. Monperrus, D. Amouroux, H. Preud'Homme, A. Prieto, O. Zuloaga, In-port derivatization coupled to different extraction techniques for the determination of alkylphenols in environmental water samples, J. Chromatogr. A. 1340 (2014) 1–7, https://doi.org/10.1016/j.chroma.2014.03.013.

[17] A. Prieto, R. Rodil, J.B. Quintana, R. Cela, M. Möder, I. Rodríguez, Evaluation of polyethersulfone performance for the microextraction of polar chlorinated herbicides from environmental water samples, Talanta 122 (2014) 264–271, https://doi.org/10.1016/j.talanta.2014.01.024.

[18] O. Ros, J.K. Izaguirre, M. Olivares, C. Bizarro, M. Ortiz-Zarragoitia, M. P. Cajaraville, N. Etxebarria, A. Prieto, A. Vallejo, Determination of endocrine disrupting compounds and their metabolites in fish bile, Sci. Total Environ. 536 (2015) 261–267, https://doi.org/10.1016/j.scitotenv.2015.07.074.

[19] O. Ros, A. Vallejo, L. Blanco-Zubiaguirre, M. Olivares, A. Delgado, N. Etxebarria, A. Prieto, Microextraction with polyethersulfone for bisphenol-A, alkylphenols and hormones determination in water samples by means of gas chromatography-mass spectrometry and liquid chromatography-tandem mass spectrometry analysis, Talanta 134 (2015) 247–255, https://doi.org/10.1016/j.talanta.2014.11.015.

[20] L. Mijangos, H. Ziarrusta, M. Olivares, O. Zuloaga, M. Möder, N. Etxebarria, A. Prieto, Simultaneous determination of 41 multiclass organic pollutants in environmental waters by means of polyethersulfone microextraction followed by liquid chromatography–tandem mass spectrometry, Anal. Bioanal. Chem. 410 (2018) 615–632, https://doi.org/10.1007/s00216-017-0763-2.

[21] O. Ros, J. Aguirre, A. Prieto, M. Olivares, N. Etxebarria, A. Vallejo, Simultaneous enzymatic hydrolysis and extraction of endocrine-disrupting chemicals in fish bile using polyethersulfone polymer, Anal. Bioanal. Chem. 407 (2015) 7413–7423, https://doi.org/10.1007/s00216-015-8905-x.

[22] L. Mijangos, H. Ziarrusta, I. Zabaleta, A. Usobiaga, M. Olivares, O. Zuloaga, N. Etxebarria, A. Prieto, Multiresidue analytical method for the determination of 41 multiclass organic pollutants in mussel and fish tissues and biofluids by liquid chromatography coupled to tandem mass spectrometry, Anal. Bioanal. Chem. 411 (2019) 493–506, https://doi.org/10.1007/s00216-018-1474-z.

[23] D.A. Alvarez, J.N. Huckins, J.D. Petty, T. Jones-Lepp, F. Stuer-Lauridsen, D.T. Getting, J.P. Goddard, A. Gravell, Chapter 8 Tool for monitoring hydrophilic contaminants in water: polar organic chemical integrative sampler (POCIS), Compr. Anal. Chem. 48 (2007) 171–197. 10.1016/S0166-526X(06)48008-9.

[24] M. Caban, H. Lis, P. Stepnowski, Limitations of Integrative Passive Samplers as a Tool for the Quantification of Pharmaceuticals in the Environment – A Critical Review with the Latest Innovations, Crit. Rev. Anal. Chem. 52 (2021) 1386–1407, https://doi.org/10.1080/10408347.2021.1881755.

[25] V. Glanzmann, K. Booij, N. Reymond, C. Weyermann, N. Estoppey, Determining the Mass Transfer Coefficient of the Water Boundary Layer at the Surface of Aquatic Integrative Passive Samplers, Environ. Sci. Technol. (2021), https://doi.org/10.1021/acs.est.1c08088.

[26] V. Fauvelle, S.L. Kaserzon, N. Montero, S. Lissalde, I.J. Allan, G. Mills, N. Mazzella, J.F. Mueller, K. Booij, Dealing with Flow Effects on the Uptake of Polar Compounds by Passive Samplers, Environ. Sci. Technol. 51 (2017) 2536–2537, https://doi.org/10.1021/acs.est.7b00558.

[27] C. Harman, I.J. Allan, P.S. Bäuerlein, The challenge of exposure correction for polar passive samplers the PRC and the POCIS, Environ. Sci. Technol. 45 (2011) 9120–9121, https://doi.org/10.1021/es2033789.

[28] K. Booij, F. Smedes, I.J. Allan, Guidelines for determining polymer-water and polymer-polymer partition coefficients of organic compounds., 2017. http://hdl.handle.net/11329/700.

[29] J. Kwon, T. Wuethrich, P. Mayer, B.I. Escher, Partition Coefficients of Highly Hydrophobic Chemicals between Poly (dimethylsiloxane) and Water, Anal. Chem. 79 (2007) 6816–6822.

[30] T. Zhu, C.T. Jafvert, D. Fu, Y. Hu, A novel method for measuring polymer-water partition coefficients, Chemosphere 138 (2015) 973–979, https://doi.org/10.1016/j.chemosphere.2014.12.040.

[31] S. Suchana, E. Passeport, Implications of Polar Organic Chemical Integrative Sampler for High Membrane Sorption and Suitability of Polyethersulfone as a Single-Phase Sampler, Sci. Total Environ. 850 (2022) 157898, https://doi.org/10.2139/ssrn.3985472.

[32] E.L.M. Vermeirssen, C. Dietschweiler, B.I. Escher, J. Van Der Voet, J. Hollender, Transfer kinetics of polar organic compounds over polyethersulfone membranes in the passive samplers pocis and chemcatcher, Environ. Sci. Technol. 46 (2012) 6759–6766, https://doi.org/10.1021/es3007854.

[33] S.L. Kaserzon, D.W. Hawker, K. Kennedy, M. Bartkow, S. Carter, K. Booij, J. F. Mueller, Characterisation and comparison of the uptake of ionizable and polar pesticides, pharmaceuticals and personal care products by POCIS and Chemcatchers, Environ. Sci. Process. Impacts. 16 (2014) 2517–2526, https://doi.org/10.1039/c4em00392f.

[34] L. Silvani, C. Riccardi, E. Eek, M.P. Papini, N.A.O. Morin, G. Cornelissen, A.M. P. Oen, S.E. Hale, Monitoring alkylphenols in water using the polar organic chemical integrative sampler (POCIS): Determining sampling rates via the extraction of PES membranes and Oasis beads, Chemosphere 184 (2017) 1362–1371, https://doi.org/10.1016/j.chemosphere.2017.06.083.

[35] S. Endo, Y. Matsuura, Characterizing Sorption and Permeation Properties of Membrane Filters Used for Aquatic Integrative Passive Samplers, Environ. Sci. Technol. 52 (2018) 2118–2125, https://doi.org/10.1021/acs.est.7b05144.

[36] N.A.O. Morin, N. Mazzella, H.P.H. Arp, J. Randon, J. Camilleri, L. Wiest, M. Coquery, C. Miège, Kinetic accumulation processes and models for 43 micropollutants in "pharmaceutical" POCIS, Sci. Total Environ. 615 (2018) 197–207, https://doi.org/10.1016/j.scitotenv.2017.08.311.

[37] Y. Jeong, A. Schäffer, K. Smith, A comparison of equilibrium and kinetic passive sampling for the monitoring of aquatic organic contaminants in German rivers, Water Res. 145 (2018) 248–258, https://doi.org/10.1016/j.watres.2018.08.016.

[38] Y. Li, C. Yang, D. Zha, L. Wang, G. Lu, Q. Sun, D. Wu, In situ calibration of polar organic chemical integrative samplers to monitor organophosphate flame retardants in river water using polyethersulfone membranes with performance reference compounds, Sci. Total Environ. 610–611 (2018) 1356–1363, https://doi.org/10.1016/j.scitotenv.2017.08.234.

[39] N. Estoppey, J. Mathieu, E. Gascon Diez, E. Sapin, O. Delémont, P. Esseiva, L.F. de Alencastro, S. Coudret, P. Folly, Monitoring of explosive residues in lake-bottom water using Polar Organic Chemical Integrative Sampler (POCIS) and chemcatcher: determination of transfer kinetics through Polyethersulfone (PES) membrane is crucial, Environ. Pollut. 252 (2019) 767–776, https://doi.org/10.1016/j.envpol.2019.04.087.

[40] V.T. Djomte, S. Chen, C.K. Chambliss, Effects of suspended sediment on POCIS sampling rates, Chemosphere 241 (2020) 124972, https://doi.org/10.1016/j.chemosphere.2019.124972.

[41] L. Wang, R. Liu, Y. Zhou, P. Yuan, X. Liu, H. Gao, Mass transfer characteristics of chiral pharmaceuticals on membrane used for polar organic chemical integrative sampler, J. Environ. Sci. (china) 136 (2024) 670–681, https://doi.org/10.1016/j.jes.2023.02.038.

[42] Y. Jeong, A. Schäffer, K. Smith, Comparison of the sampling rates and partitioning behaviour of polar and non-polar contaminants in the polar organic chemical integrative sampler and a monophasic mixed polymer sampler for application as an equilibrium passive sampler, Sci. Total Environ. 627 (2018) 905–915, https://doi.org/10.1016/j.scitotenv.2018.01.273.

[43] A.T.K. Tran, R.V. Hyne, P. Doble, Calibration of a passive sampling device for time-integrated sampling of hydrophilic herbicides in aquatic environments, Environ. Toxicol. Chem. 26 (2007) 435–443, https://doi.org/10.1897/06-401R.1.

[44] V. Glanzmann, N. Reymond, C. Weyermann, N. Estoppey, An improved Chemcatcher-based method for the integrative passive sampling of 44 hydrophilic micropollutants in surface water – Part A: Calibration under four controlled hydrodynamic conditions, Sci. Total Environ. 871 (2023) 162037, https://doi.org/10.1016/j.scitotenv.2023.162037.

[45] H. MacKeown, E. Magi, M. Di Carro, B. Benedetti, Unravelling the role of membrane pore size in polar organic chemical integrative samplers (POCIS) to broaden the polarity range of sampled analytes, Anal. Bioanal. Chem. 414 (2022) 1963–1972, https://doi.org/10.1007/s00216-021-03832-4.

[46] A. Seen, O. Bizeau, L. Sadler, T. Jordan, D. Nichols, Assessment of Envi-Carb^{TM} as a passive sampler binding phase for acid herbicides without pH adjustment, Chemosphere 103 (2014) 306–312, https://doi.org/10.1016/j.chemosphere.2013.11.075.

[47] I. Townsend, L. Jones, M. Broom, A. Gravell, M. Schumacher, G.R. Fones, R. Greenwood, G.A. Mills, Calibration and application of the Chemcatcher® passive sampler for monitoring acidic herbicides in the River Exe, UK catchment, Environ. Sci. Pollut. Res. 25 (2018) 25130–25142, https://doi.org/10.1007/s11356-018-2556-3.

[48] M. Godere, S. Mondange, P. Doumenq, C. Gonzalez, L. Malleret, First study of passive sampling to monitor short-chain chlorinated paraffins in water: Comparing capabilities of Chemcatcher® and silicone rubber samplers, Talanta 224 (2021) 121920, https://doi.org/10.1016/j.talanta.2020.121920.

[49] B. Becker, C. Kochleus, D. Spira, J. Bachtin, F. König, S. Meinecke, C. Möhlenkamp, K. Booij, Modelling passive sampling of hydrophilic compounds under time-variable aqueous concentrations, Environ. Sci. Pollut. Res. 31 (2024) 51844–51857, https://doi.org/10.1007/s11356-024-34460-x.

[50] B. Becker, C. Kochleus, D. Spira, C. Möhlenkamp, J. Bachtin, S. Meinecke, E.L. M. Vermeirssen, Passive sampler phases for pesticides: evaluation of AttractSPE^{TM} SDB-RPS and HLB versus Empore^{TM} SDB-RPS, Environ. Sci. Pollut. Res. 28 (2021) 11697–11707, https://doi.org/10.1007/s11356-020-12109-9.

[51] Y. Jeong, H.A. Kwon, H.P. Jeon, A. Schäffer, K. Smith, Quantitative evaluation of polyethersulfone and polytetrafluoroethylene membrane sorption in a polar organic chemical integrative sampler (POCIS), Environ. Pollut. 266 (2020), https://doi.org/10.1016/j.envpol.2020.115224.

[52] S.L. Kaserzon, E.L.M. Vermeirssen, D.W. Hawker, K. Kennedy, C. Bentley, J. Thompson, K. Booij, J.F. Mueller, Passive sampling of perfluorinated chemicals in water: Flow rate effects on chemical uptake, Environ. Pollut. 177 (2013) 58–63, https://doi.org/10.1016/j.envpol.2013.02.002.

[53] A. Togola, H. Budzinski, Development of polar organic integrative samplers for analysis of pharmaceuticals in aquatic systems, Anal. Chem. 79 (2007) 6734–6741, https://doi.org/10.1021/ac070559i.

[54] S.L. Kaserzon, K. Kennedy, D.W. Hawker, J. Thompson, S. Carter, A.C. Roach, K. Booij, J.F. Mueller, Development and calibration of a passive sampler for perfluorinated alkyl carboxylates and sulfonates in water, Environ. Sci. Technol. 46 (2012) 4985–4993, https://doi.org/10.1021/es300593a.

[55] S. Suchana, E. Edwards, E.E. Mack, L. Lomheim, N. Melo, S. Gavazza, E. Passeport, Compatibility of polar organic chemical integrative sampler (POCIS)

with compound specific isotope analysis (CSIA) of substituted chlorobenzenes, Sci. Total Environ. 906 (2024), https://doi.org/10.1016/j.scitotenv.2023.167628.

[56] A. Casari, L. Tonidandel, G. Zolezzi, A. Bellin, P. Negri, A. Barbero, R. Larcher, Validation of a calibration model able to estimate the concentration of pesticides in an alpine stream through passive sampling (POCIS) monitoring, Environ. Chem. (2023) 1–15, https://doi.org/10.1071/en23052.

[57] Y.Y. Liu, M. Digaletos, C.J. Ptacek, J.L. Thomas, Active and passive sampling techniques in headwater streams to characterize acesulfame-K, pharmaceutical and phosphorus contamination from on-site wastewater disposal systems in Canadian rural hamlets, Sci. Total Environ. 956 (2024) 177194, https://doi.org/10.1016/j.scitotenv.2024.177194.

[58] K. Godlewska, A. Białk-Bielińska, P. Mazierski, S. Zdybel, A. Sosnowska, D. Górzyński, T. Puzyn, A. Zaleska-Medynska, T. Klimczuk, M. Paszkiewicz, Assessment of the application of selected metal-organic frameworks as advanced sorbents in passive extraction used in the monitoring of contaminants of emerging concern in surface waters, Sci. Total Environ. 927 (2024), https://doi.org/10.1016/j.scitotenv.2024.172215.

[59] S. Lissalde, N. Mazzella, P. Mazellier, Polar organic chemical integrative samplers for pesticides monitoring: Impacts of field exposure conditions, Sci. Total Environ. 488–489 (2014) 188–196, https://doi.org/10.1016/j.scitotenv.2014.04.069.

[60] V. Castro, J.B. Quintana, I. Carpinteiro, J. Cobas, N. Carro, R. Cela, R. Rodil, Combination of different chromatographic and sampling modes for high-resolution mass spectrometric screening of organic microcontaminants in water, Anal. Bioanal. Chem. 413 (2021) 5607–5618, https://doi.org/10.1007/s00216-021-03226-6.

[61] J.B. Renaud, L. Sabourin, S. Hoogstra, P. Helm, D.R. Lapen, M.W. Sumarah, Monitoring of Environmental Contaminants in Mixed-Use Watersheds Combining Targeted and NonTargeted Analysis with Passive Sampling, Environ. Toxicol. Chem. 00 (2021) 1–13, https://doi.org/10.1002/etc.5192.

[62] H. MacKeown, C. Scapuzzi, M. Baglietto, B. Benedetti, M. Di Carro, E. Magi, Wastewater and seawater monitoring in Antarctica: Passive sampling as a powerful strategy to evaluate emerging pollution, Sci. Total Environ. 925 (2024) 171755, https://doi.org/10.1016/j.scitotenv.2024.171755.

[63] H. MacKeown, B. Benedetti, C. Scapuzzi, M. Di Carro, E. Magi, A Review on Polyethersulfone Membranes in Polar Organic Chemical Integrative Samplers: Preparation, Characterization and Innovation, Crit. Rev. Anal. Chem. (2022) 1–17, https://doi.org/10.1080/10408347.2022.2131374.

[64] B. Bonnaud, N. Mazzella, P. Boutet, A. Daval, C. Miège, Calibration comparison between two passive samplers -o-DGT and POCIS- for 109 hydrophilic emerging and priority organic compounds, Sci. Total Environ. 869 (2023) 161720, https://doi.org/10.1016/j.scitotenv.2023.161720.

[65] M. Caban, H. Męczykowska, P. Stepnowski, Application of the PASSIL technique for the passive sampling of exemplary polar contaminants (pharmaceuticals and phenolic derivatives) from water, Talanta 155 (2016) 185–192, https://doi.org/10.1016/j.talanta.2016.04.035.

[66] H. Męczykowska, P. Kobylis, P. Stepnowski, M. Caban, Ionic liquids for the passive sampling of sulfonamides from water—applicability and selectivity study, Anal. Bioanal. Chem. 409 (2017) 3951–3958, https://doi.org/10.1007/s00216-017-0342-6.

[67] B. Medon, B.G. Pautler, A. Sweett, J. Roberts, F.F. Risacher, L.A. D'Agostino, J. Conder, J.R. Gauthier, S.A. Mabury, A. Patterson, P. McIsaac, R. Mitzel, S. G. Hakimabadi, A.L.T. Pham, A field-validated equilibrium passive sampler for the monitoring of per- and polyfluoroalkyl substances (PFAS) in sediment pore water and surface water, Environ. Sci. Process. Impacts. 25 (2023) 980–995, https://doi.org/10.1039/d2em00483f.

[68] S. Endo, Y. Matsuura, E.L.M. Vermeirssen, Mechanistic Model Describing the Uptake of Chemicals by Aquatic Integrative Samplers: Comparison to Data and Implications for Improved Sampler Configurations, Environ. Sci. Technol. 53 (2019) 1482–1489, https://doi.org/10.1021/acs.est.8b06225.

[69] S.S. Liu, J.L. Li, L.K. Ge, C.L. Li, J.L. Zhao, Q.Q. Zhang, G.G. Ying, C.E. Chen, Selective diffusive gradients in thin-films with molecularly imprinted polymer for measuring fluoroquinolone antibiotics in waters, Sci. Total Environ. 790 (2021) 148194, https://doi.org/10.1016/j.scitotenv.2021.148194.

[70] Y.T. Zou, Z. Fang, Y. Li, R. Wang, H. Zhang, K.C. Jones, X.Y. Cui, X.Y. Shi, D. Yin, C. Li, Z.D. Liu, L.Q. Ma, J. Luo, Novel Method for in Situ Monitoring of Organophosphorus Flame Retardants in Waters, Anal. Chem. 90 (2018) 10016–10023, https://doi.org/10.1021/acs.analchem.8b02480.

[71] S. Ren, X. Jin, T. Girma, B. Min, L. Jing, D. Feng, T. Lingxin, Development and application of diffusive gradients in thin films for in situ sampling of the organic UV filter 4 - methylbenzylidene camphor (4 - MBC) in waters, Environ. Sci. Pollut. Res. (2023), https://doi.org/10.1007/s11356-023-28844-8.

[72] P. Wang, J. Li, M.Y. Xie, C.C. Wu, C.S. Wong, E.Y. Zeng, Utility of a modified o-DGT passive sampler for measurement of bisphenol analogues in freshwater and coastal waters, Sci. Total Environ. 931 (2024) 172978, https://doi.org/10.1016/j.scitotenv.2024.172978.

[73] W. Chen, S. Pan, H. Cheng, A.J. Sweetman, H. Zhang, K.C. Jones, Diffusive gradients in thin-films (DGT) for in situ sampling of selected endocrine disrupting chemicals (EDCs) in waters, Water Res. 137 (2018) 211–219, https://doi.org/10.1016/j.watres.2018.03.029.

[74] Q. Rong, Y. Li, J. Luo, L. Yan, K.C. Jones, H. Zhang, Development of a novel DGT passive sampler for measuring polycyclic aromatic hydrocarbons in aquatic systems, J. Hazard. Mater. 470 (2024) 134199, https://doi.org/10.1016/j.jhazmat.2024.134199.

[75] F. Dong, F. Ge, X. Zhao, D. Sun, S. Ren, Y. Wang, F. Tan, Measurement of perfluoroalkyl substances in drinking water sources by DGT sampler with a novel fluorinated graphite binding gel, Sci. Total Environ. 912 (2024) 169658, https://doi.org/10.1016/j.scitotenv.2023.169658.

[76] Y. Li, M. Wu, M. Fu, D. Tan, P. Zhang, Z. Zhou, X. Li, Validation and Application of the Diffusive Gradients in Thin-Films Technique for In Situ Measurement of β-Blocker Drugs in Waters and Sediments, Water (Switzerland) 16 (2024), https://doi.org/10.3390/w16111478.

[77] S.S. Liu, S.B. Chen, Y.B. Yue, X.H. Li, C. Zhang, G.G. Ying, C.E. Chen, Development and validation of diffusive gradients in thin-films for in situ monitoring of ionic liquids in waters, Anal. Methods. (2024), https://doi.org/10.1039/d4ay01730g.

[78] C. Guo, T. Zhang, S. Hou, J. Lv, Y. Zhang, F. Wu, Z. Hua, W. Meng, H. Zhang, J. Xu, Investigation and Application of a New Passive Sampling Technique for in Situ Monitoring of Illicit Drugs in Waste Waters and Rivers, Environ. Sci. Technol. 51 (2017) 9101–9108, https://doi.org/10.1021/acs.est.7b00731.

[79] W. Chen, Y. Li, C.E. Chen, A.J. Sweetman, H. Zhang, K.C. Jones, DGT Passive Sampling for Quantitative in Situ Measurements of Compounds from Household and Personal Care Products in Waters, Environ. Sci. Technol. 51 (2017) 13274–13281, https://doi.org/10.1021/acs.est.7b03940.

[80] J.L. Zheng, D.X. Guan, J. Luo, H. Zhang, W. Davison, X.Y. Cui, L.H. Wang, L. Q. Ma, Activated charcoal based diffusive gradients in thin films for in situ monitoring of bisphenols in waters, Anal. Chem. 87 (2015) 801–807, https://doi.org/10.1021/ac503814j.

[81] R. Wang, Y. Zou, J. Luo, K.C. Jones, H. Zhang, Investigating Potential Limitations of Current Diffusive Gradients in Thin Films (DGT) Samplers for Measuring Organic Chemicals, Anal. Chem. 91 (2019) 12835–12843, https://doi.org/10.1021/acs.analchem.9b02571.

[82] Y. Zhu, G. Xu, X. Wang, X. Ji, X. Jia, L. Sun, X. Gu, X. Xie, Passive sampling of chlorophenols in water and soils using diffusive gradients in thin films based on β-cyclodextrin polymers, Sci. Total Environ. 806 (2022) 150739, https://doi.org/10.1016/j.scitotenv.2021.150739.

[83] D.X. Guan, Y.Q. Li, N.Y. Yu, G.H. Yu, S. Wei, H. Zhang, W. Davison, X.Y. Cui, L. Q. Ma, J. Luo, In situ measurement of perfluoroalkyl substances in aquatic systems using diffusive gradients in thin-films technique, Water Res. 144 (2018) 162–171, https://doi.org/10.1016/j.watres.2018.07.031.

[84] Y. Zhang, T. Zhang, C. Guo, S. Hou, Z. Hua, J. Lv, Y. Zhang, J. Xu, Development and application of the diffusive gradients in thin films technique for simultaneous measurement of methcathinone and ephedrine in surface river water, Sci. Total Environ. 618 (2018) 284–290, https://doi.org/10.1016/j.scitotenv.2017.11.068.

[85] R. Martins de Barros, S. Lissalde, R. Guibal, G. Guibaud, Adaptation of the o-DGT for the sampling of 12 hormones: calibration, performance evaluation, and recommendation, Environ. Sci. Pollut. Res. 30 (2023) 68177–68190, https://doi.org/10.1007/s11356-023-26975-6.

[86] H. Ijaz, J.X. Zi, S.S. Liu, Q.S. Cai, S.M. Cheng, Z.X. Zhao, G.G. Ying, A. J. Sweetman, C.E. Chen, Development of diffusive gradients in thin-films with mixed binding gels for in situ monitoring of artificial sweeteners in waters, Environ. Sci. Adv. 2 (2023), https://doi.org/10.1039/d2va00320a.

[87] X. Ji, J.K. Challis, M. Brinkmann, A critical review of diffusive gradients in thin films technique for measuring organic pollutants: Potential limitations, application to solid phases, and combination with bioassays, Chemosphere 287 (2022) 132352, https://doi.org/10.1016/j.chemosphere.2021.132352.

[88] K. Godlewska, P. Stepnowski, M. Paszkiewicz, Carbon nanotubes, activated carbon and Oasis HLB as sorbents of passive samplers for extraction of selected micropollutants — Comparison of sampling rates and extraction efficiency, Microchem. J. 172 (2022) 106975, https://doi.org/10.1016/j.microc.2021.106975.

[89] M. Vinyes-Nadal, J. Masbou, S. Kümmel, M. Gehre, G. Imfeld, N. Otero, C. Torrentó, Novel extraction methods and compound-specific isotope analysis of methoxychlor in environmental water and aquifer slurry samples, Sci. Total Environ. 931 (2024), https://doi.org/10.1016/j.scitotenv.2024.172858.

[90] C.N. Manners, D.W. Payling, D.A. Smith, Distribution coefficient, a convenient term for the relation of predictable physico-chemical properties to metabolic processes, Xenobiotica 18 (1988) 331–350, https://doi.org/10.3109/00498258809041669.

[91] R.A. Scherrer, S.M. Howard, Use of Distribution Coefficients in Quantitative Structure-Activity Relationships, J. Med. Chem. 20 (1977) 53–58, https://doi.org/10.1021/jm00211a010.

[92] R.E. Plummer, C.J. Hapeman, P. Rice, G.W. Mccarty, W.F. Schmidt, P.M. Downey, T.B. Moorman, E.A. Douglas, T.C. Strickland, O. Pisani, D.D. Bosch, K.R. Elkin, A. R. Buda, Method to Evaluate the Age of Groundwater Inputs to Surface Waters by Determining the Chirality Change of Metolachlor Ethanesulfonic Acid (MESA) Captured on a Polar Organic Chemical Integrative Sampler (POCIS) The United States Environmental Protectio, J. Agric. Food Chem. 68 (2020) 2297–2305, https://doi.org/10.1021/acs.jafc.9b06187.

[93] S.L. MacLeod, E.L. McClure, C.S. Wong, Laboratory calibration and field deployment of the polar organic chemical integrative sampler for pharmaceuticals and personal care products in wastewater and surface water, Environ. Toxicol. Chem. 26 (2007) 2517–2529, https://doi.org/10.1897/07-238.1.

[94] A. Arditsoglou, D. Voutsa, Passive sampling of selected endocrine disrupting compounds using polar organic chemical integrative samplers, Environ. Pollut. 156 (2008) 316–324, https://doi.org/10.1016/j.envpol.2008.02.007.

[95] E.L.M. Vermeirssen, O. Körner, R. Schönenberger, M.J.F. Suter, P. Burkhardt-Holm, Characterization of environmental estrogens in river water using a three pronged approach: Active and passive water sampling and the analysis of

accumulated estrogens in the bile of caged fish, Environ. Sci. Technol. 39 (2005) 8191–8198, https://doi.org/10.1021/es050818q.

[96] R.Z. Hahn, M.F. Bastiani, L. de Lima Feltraco Lizot, I.C. da Silva Moreira, Y. F. Meireles, A. Schneider, C.A. do Nascimento, R. Linden, Determination of a comprehensive set of drugs of abuse, metabolites and human biomarkers in wastewater using passive sampling followed by UHPLC-MS/MS analysis, Microchem. J. 172 (2022) 106960, https://doi.org/10.1016/j.microc.2021.106960.

[97] J.C. Carlson, J.K. Challis, M.L. Hanson, C.S. Wong, Stability of pharmaceuticals and other polar organic compounds stored on polar organic chemical integrative samplers and solid-phase extraction cartridges, Environ. Toxicol. Chem. 32 (2013) 337–344, https://doi.org/10.1002/etc.2076.

[98] A. Rico, A. Arenas-Sánchez, C. Alonso-Alonso, I. López-Heras, L. Nozal, D. Rivas-Tabares, M. Vighi, Identification of contaminants of concern in the upper Tagus river basin (central Spain). Part 1: Screening, quantitative analysis and comparison of sampling methods, Sci. Total Environ. 666 (2019) 1058–1070, https://doi.org/10.1016/j.scitotenv.2019.02.250.

[99] J.K. Challis, K.M. Stroski, K.H. Luong, M.L. Hanson, C.S. Wong, Field Evaluation and in Situ Stress Testing of the Organic-Diffusive Gradients in Thin-Films Passive Sampler, Environ. Sci. Technol. 52 (2018) 12573–12582, https://doi.org/10.1021/acs.est.8b03622.

[100] L. de Lima Feltraco Lizot, M.F. Bastiani, R.Z. Hahn, Y.F. Meireles, M. Freitas, C.A. do Nascimento, R. Linden, Determination of the pyrethroid inseticide metabolite 3-phenoxybenzoic acid in wastewater using polar organic integrative samplers and LC-MS/MS analysis, Microchem. J. 190 (2023) 108574. 10.1016/j.microc.2023.108574.

[101] H. Lis, P. Stepnowski, M. Caban, Static renewal and continuous-flow calibration of two types of passive samplers for the monitoring of pharmaceuticals in wastewater, Microchem. J. 165 (2021) 106121, https://doi.org/10.1016/j.microc.2021.106121.

[102] H. Nyoni, L. Chimuka, B. Vrana, E. Cukrowska, Membrane assisted passive sampler for triazine compounds in water bodies-Characterization of environmental conditions and field performance, Anal. Chim. Acta. 694 (2011) 75–82, https://doi.org/10.1016/j.aca.2011.03.045.

[103] K.J. Hageman, C.H.F. Aebig, K.H. Luong, S.L. Kaserzon, C.S. Wong, T. Reeks, M. Greenwood, S. Macaulay, C.D. Matthaei, Current-use pesticides in New Zealand streams: Comparing results from grab samples and three types of passive samplers, Environ. Pollut. 254 (2019) 112973, https://doi.org/10.1016/j.envpol.2019.112973.

[104] L. Mijangos, O. Urain, L. Ruiz-Rubio, H. Ziarrusta, M. Olivares, O. Zuloaga, A. Prieto, N. Etxebarria, Short-term stability assessment for the analysis of emerging contaminants in seawater, Environ. Sci. Pollut. Res. 26 (2019) 23861–23872, https://doi.org/10.1007/s11356-019-05172-4.

[105] K. Godlewska, P. Stepnowski, M. Paszkiewicz. Pollutant analysis using passive samplers: principles, sorbents, calibration and applications. A review, Springer International Publishing, 2021, https://doi.org/10.1007/s10311-020-01079-6.

[106] H. MacKeown, B. Benedetti, M. Di Carro, E. Magi, The study of polar emerging contaminants in seawater by passive sampling : A review, Chemosphere 299 (2022) 134448, https://doi.org/10.1016/j.chemosphere.2022.134448.

[107] K. Booij, B. Vrana, J.N. Huckins, Chapter 7 Theory, modelling and calibration of passive samplers used in water monitoring, Compr. Anal. Chem. 48 (2007) 141–169, https://doi.org/10.1016/S0166-526X(06)48007-7.

[108] J.N. Huckins, K. Booij, J.D. Petty. Monitors of Organic Chemicals in the Environment, Springer, New York, NY, 2006, https://doi.org/10.1007/0-387-35414-x.