


# Measuring the exposome: a practical guide for using wearable passive samplers to assess environmental influences

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## Abstract

Wearable passive samplers present tremendous opportunity for measuring the exposome. These tools offer a user-friendly and cost-effective approach to assess personal exposure, enabling access to remote communities and under-researched vulnerable populations. Use of these wearable devices has gained popularity over the past two decades but before these tools can be adopted for routine use in large-scale health studies, they require standardization to ensure data reproducibility. With the objective of harmonizing wearable passive sampler use, this paper serves as a guide to available technologies (Fresh Air samplers, commercial silicone wristbands, custom silicone bands, and the silicone brooch) and best practices for assessing exposure to environmental chemicals. We discuss the optimal duration to wear these sampling tools, essential quality control and quality assurance measures, chemical analysis approaches, and strategies to interpret measured exposures. We also propose minimum guidelines for sample collection and reporting data to foster measurement standardization and secondary analysis. Strategies to improve data transparency through harmonization will enable comparability of the comprehensive measures of the exposome using wearable passive samplers.

**Key words:** exposome; wristbands; wearable passive samplers; personal exposure; mass spectrometry; chemical.

## Background

The exposome encompasses all environmental influences that shape health throughout life, including what we eat and do, as well as where we live and work.<sup>1</sup> Measuring the exposome requires innovative approaches that capture our multifaceted exposure patterns. Environmental matrices such as air, water, and settled dust can assess exposome features.<sup>2–4</sup> Air serves as an integrative sink for capturing exposures from diverse environmental sources through both direct emissions from vehicles, industry, and cooking, and volatilization from consumer products, furnishings, building materials, and food products.<sup>5–8</sup> Exposure to airborne contaminants can be assessed through two primary approaches: active sampling, which relies on pumps to draw air through collection media, and passive sampling, which operates without pumps.<sup>9–11</sup> Wearable passive samplers represent an emerging advancement for personalizing exposure measurements.<sup>9–11</sup> These devices enable continuous, unobtrusive monitoring of individual exposures across the multiple microenvironments people encounter in their daily lives. When integrated with high-resolution mass spectrometry, wearable passive samplers enable extensive characterization of external chemical

and biological stressors at an omics scale, facilitating discovery of novel environmental risk factors.

Passive air sampling has been utilized since the 1970s to characterize environmental exposures.<sup>12–15</sup> These samplers offer significant advantages over traditional active sampler by eliminating the need for power, thereby reducing cost, weight, size, and noise.<sup>12,13,16</sup> The lightweight design of wearable passive samplers promotes better compliance during routine daily activities, particularly amongst vulnerable populations.<sup>12,13,16,17</sup> This versatility has enabled their use across a broad range of studies, including characterizing temporal and spatial chemical distributions across different environments, examining variability within and between populations, tracking longitudinal exposures throughout the life course from infancy to adulthood,<sup>18–21</sup> and evaluating the influence on health and disease.<sup>22–24</sup>

Despite their simple design, wearable passive samplers rely on complex underlying mechanisms, and numerous factors can influence their performance.<sup>12</sup> The increasing use of these tools for evaluating personal exposures necessitates standardized sample collection and analysis approaches to enable quantitative assessment and ensure data reproducibility.

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The objective of this paper is to provide comprehensive guidance for implementing wearable passive samplers in exposome studies. Drawing on our experience developing and working with wearable passive samplers over the past decade, we address frequently asked questions about wearable passive samplers, covering sampler design, sampling theory, calibration, field deployment, preparation, data acquisition, and interpretation. Additionally, we propose standardized framework for collecting, processing and analyzing wearable passive samplers to facilitate comparability across laboratories. The paper is a much-needed resource that lowers the barrier for those seeking to use wearable passive samplers in exposome research.

## Wearable passive sampler designs and personal exposure assessment

### Question 1.1 What are wearable passive samplers?

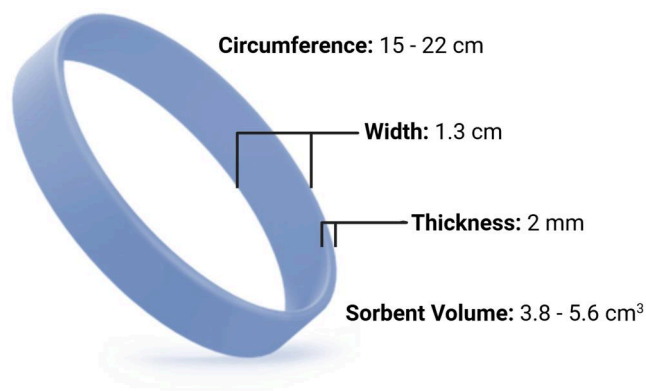
Wearable passive samplers are tools for evaluating personal exposure to environmental contaminants. The range of contaminants that have been assessed using passive samplers include inorganic gases (eg, ozone,<sup>25,26</sup> nitrogen dioxide,<sup>27,28</sup> sulfur dioxide<sup>29</sup>), volatile organic compounds (VOCs),<sup>30,31</sup> semi-volatile organic compounds (SVOCs<sup>32</sup>), particles (eg, metals,<sup>33</sup> black carbon,<sup>34,35</sup> microplastics<sup>36</sup>), and pathogens (bacteria, fungi, viruses).<sup>37,38</sup> The various airborne phases of compounds are further discussed in Question 1.3. Passive samplers contain sorbent materials (eg, silicone rubber, polyurethane foam, fabric, glass fiber filter) that accumulates contaminants through diffusion and deposition.<sup>13,39,40</sup> When worn, these devices collect exposure arising from an individual's activities across the unique combination of indoor and outdoor environments they frequent. Wearable passive samplers used in exposomic and environmental health studies include mini-polyurethane foam (PUF),<sup>41</sup> silicone bands,<sup>17,42</sup> custom silicone bands,<sup>23</sup> Fresh Air samplers, and the brooch.<sup>43</sup> Apart from the mini-PUF reported once in the literature, all these commonly used devices employ polydimethylsiloxane (PDMS), also known as silicone rubber, as their primary sorbent (PDMS and silicone rubber are used interchangeably in this paper and in the literature.). Each design incorporates distinctive features that influence both the dynamics of contaminant collection and the source of captured contaminants—air, skin, or both. Our previous paper compared different designs of PDMS-based wearable samplers, including their calibration status, advantages and disadvantages and scope of applicability.<sup>9</sup> Here, we briefly describe the four PDMS devices as examples of commonly used wearable passive samplers.

#### Commercial silicone bands

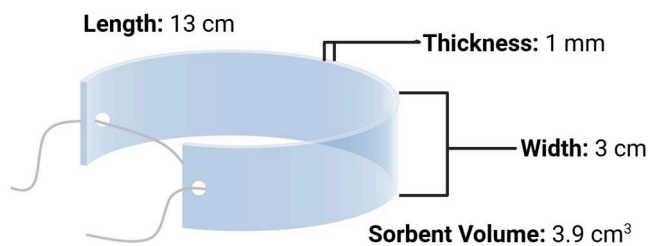
These samplers are flexible loops of colored silicone rubber that are commercially available as awareness bands (Figure 1). The bands are available in a range of sizes to fit a wide age range. Silicone bands have most commonly been worn on the wrist or ankle to capture a contaminants from the air and skin.<sup>17,42</sup>

#### Custom silicone bands

This wearable passive sampler consists of a translucent strip of PDMS (Specialty Silicone Products, Inc., Ballston Spa, NY) (Figure 2). This material is a higher purity silicone compared to the commercial silicone bands. This design has been worn on the wrist or upper arm in studies<sup>23,44</sup> to capture contaminants from both air and skin.



**Figure 1.** Silicone bands are commercially available in various colors from multiple suppliers (eg, 24hourwristbands.com).



**Figure 2.** Custom silicone band wearable passive samplers are made from a translucent loop of PDMS that is fastened to a person's wrist or arm with a piece of string.

#### Fresh air samplers

Fresh Air samplers consist of a wearable attachment and a perforated polytetrafluoroethylene (PTFE) housing case containing replicate PDMS sorbent bars (Figure 3A).<sup>11</sup> The PDMS sorbent bars are custom-fabricated glass tubes coated with PDMS. These samplers are available in different designs, including silicone (Figure 3B) and nylon/Velcro bands (Figure 3C) for wearing on the wrist or ankle, as well as a magnetic clip for attachment to shirt collars, shoes, or bags (Figure 3D).<sup>16</sup> By housing the sorbent within the protective case, Fresh Air samplers exclusively collect gas-phase contaminants.

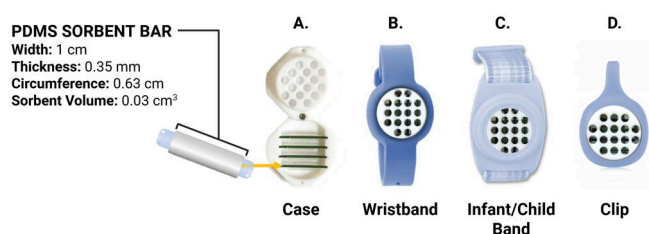
#### Brooch

This wearable passive sampler consists of a translucent PDMS sheet (Specialty Silicone Products, Inc., Ballston Spa, NY) stapled to an aluminum support<sup>23,43,45</sup> (Figure 4). Using safety pins, the brooch sampler is attached to clothing in the breathing zone to capture contaminants from the air.

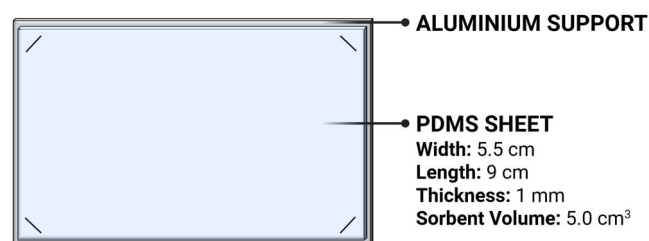
The various designs of wearable passive samplers provide different wearable forms to suit the needs of the study population and location. For example, some designs are more suitable for use with infants/children (eg, Fresh Air sampler) whilst others are designed for adults (eg, the brooch sampler). Note that some passive samplers, such as Fresh Air samplers, shelter the sorbent within a housing chamber. This sheltering is useful for eliminating direct contact with surfaces (skin, garments, textiles), regulating wind speed entering the sampler, and maintaining constant uptake rates.<sup>9</sup>

### Question 1.2 How do exposure levels compare between the different designs of wearable passive samplers?

Exposure profiles and levels captured using different designs of wearable passive samplers can vary depending on deployment



**Figure 3.** The Fresh Air sampler uses (A) PDMS sorbent bars to collect environmental contaminants. Up to four replicate sorbent bars are housed within (B) a perforated case that can be worn using various designs: (C) silicone band, (D) nylon/Velcro band, or (E) magnetic clip.



**Figure 4.** The brooch wearable passive sampler consists of a PDMS sheet stapled to custom-cut aluminum support.

location on the body. For example, Fresh Air samplers worn on the face, chest, wrist, and shoe generated comparable exposures for the wrist and chest samplers while face and the foot samplers differed significantly.<sup>16,46</sup> Another study comparing brooches worn on the chest and custom bands worn on the wristband and arm found exposures were correlated for less than 15% of assessed chemicals. The differences in exposure estimates reflect distinct uptake mechanisms. Fresh Air samplers are designed with a protective housing that limits collection to airborne compounds, whereas exposed silicone bands accumulate chemicals from multiple pathways including atmospheric uptake and transfer from contacted surfaces such as skin. These findings show that the research question or objective should guide the choice of sampler design and deployment location.

### Question 1.3 What environmental factors can be assessed using wearable passive samplers?

Wearable passive samplers can be used to assess a diverse range of chemical and biological contaminants. Depending on the analytical approach used, known exposures of concern can be quantified as volumetric concentrations (ie,  $\text{ng}/\text{m}^3$ ) while emerging or previously unknown contaminants can be screened and reported as semi-quantitative or qualitative estimates of exposure (See Question 3.1-3.4). Chemical contaminants include volatile inorganic compounds, VOCs, SVOCs, and particles. Volatile inorganic compounds (eg, nitrogen dioxide, sulfur dioxide, and ozone<sup>9,10</sup>) commonly exist as gases at room temperature and pressure. VOCs (eg, hexane, toluene, benzene, and formaldehyde) are liquids that easily vaporize into gases at room temperature and pressure. SVOCs are typically liquids or solids that can vaporize to stay as gases as well as become attached to particles at room temperature and pressure.<sup>2,45</sup> Common examples of SVOCs are polycyclic aromatic hydrocarbons (PAHs), polybrominated diphenyl ethers (PBDEs), novel brominated flame retardants (NBFRs), chlorinated flame retardants (CRFs), organophosphates (OPEs), and per- and polyfluoroalkyl substances (PFAS).<sup>9</sup> VOCs and SVOCs are classified based on their volatility—a measure of how easily they evaporate into a gas at a given temperature.

Various classification schemes exist for categorizing chemicals as VOCs or SVOCs, including molecular weight, saturation mass concentration, or vapor pressure. At room temperature, the vapor pressures are above  $10^{-2}$  kPa for VOCs and the range of  $10^{-2}$  to  $10^{-8}$  kPa for SVOCs.<sup>47</sup> Particle contaminants are usually mixtures including black carbon,<sup>34</sup> metals,<sup>33</sup> microplastics,<sup>36</sup> and water.<sup>48</sup> Wearable passive samplers can also be used to assess exposure to biological contaminants, including virus-laden particles such as SARS-CoV-2, fungi, and bacteria-containing droplets or particles (see Angel et al. 2022 for summary).<sup>38</sup> The ability of wearable passive samplers to capture a broad spectrum of small molecules make these tools attractive for measuring the exposome.

## Fundamentals of passive sampling

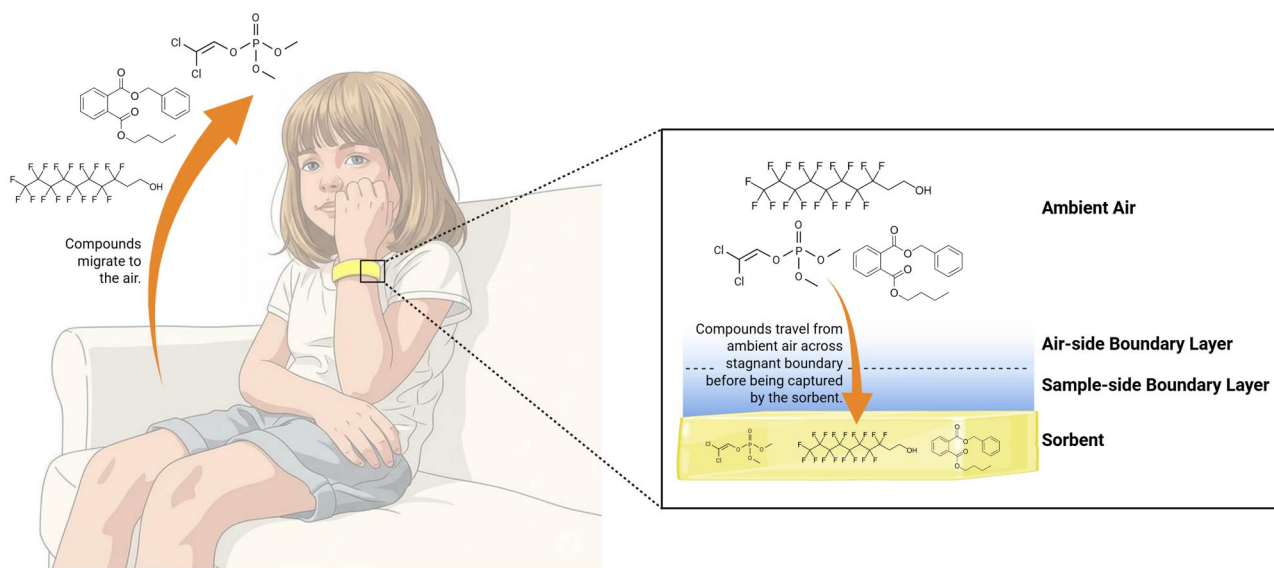
### Question 2.1 How do wearable passive samplers collect environmental contaminants?

Wearable passive samplers collect environmental contaminants by diffusion and deposition. Understanding the theory of passive sampling helps determine how long samplers should be worn and how exposure concentrations are calculated. The sorbent of a wearable passive sampler is surrounded by a stagnant boundary layer between the sorbent and air.<sup>13</sup> As the sampler is worn, smaller molecules (gases and gas-phase chemicals) primarily diffuse from the air across this stagnant boundary layer before being captured by the sorbent, while larger particles and particle-bound compounds directly deposit (gravitational settling, impaction) on the sorbent (Figure 5).<sup>12,13,40</sup>

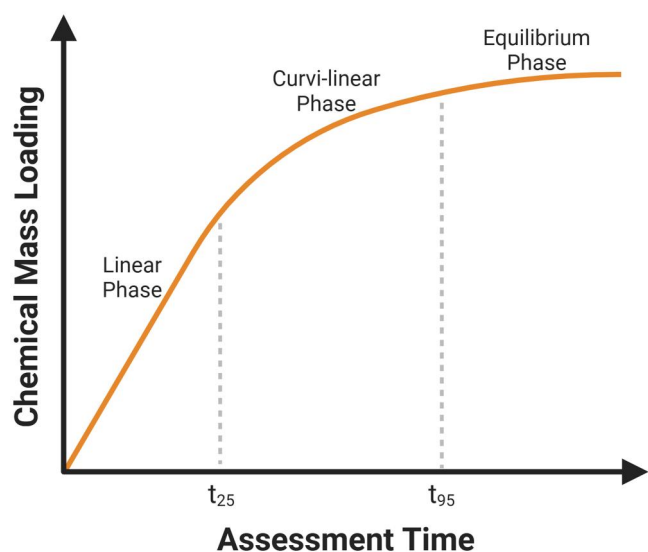
The uptake of chemicals from the air via diffusion follows three distinct phases: linear, curvi-linear, and equilibrium (Figure 6).<sup>12,13,38,40,49</sup> Initially, wearable passive samplers collect these contaminants in the *linear uptake phase*, which continues until the sampler reaches 25% of its equilibrium capacity ( $t_{25}$ ). During this phase, chemicals must overcome the resistance of the stagnant boundary layer over the sorbent.<sup>12,13</sup> The uptake rate is controlled by the air-side resistance of the boundary layer, characterized by the mass transfer coefficient.<sup>12,13</sup> The *curvi-linear phase* occurs between 25%-95% capacity ( $t_{25}$  to  $t_{95}$ ), during which the uptake rate decreases compared to the linear phase. In the *equilibrium phase* (beyond  $t_{95}$ ), the uptake rate equals the loss rate of chemicals to the air, and uptake is governed by the chemical's affinity for the sorbent (ie, sorbent-air partition ratio). This collection mechanism is termed equilibrium sampling. In contrast to the linear phase, boundary layer resistance on the sampler side controls uptake in both the curvi-linear and equilibrium phases.<sup>12,13</sup>

While uptake profiles for gases and gas-phase chemicals have been well-characterized, understanding of particle and particle-phase contaminant uptake—including organics, biologicals, metals, and microplastics—remains limited.<sup>38</sup> Under controlled conditions, particles and particle-bound compounds typically follow a linear uptake pattern when depositing onto passive sampling surfaces, particularly when surface saturation is minimal and airborne concentrations remain relatively constant.<sup>38</sup>

Uptake profiles can be determined through calibration studies or theoretically estimation.<sup>38,43</sup> Calibration studies involve deploying co-located active and passive samplers over multiple days, then measuring collected compounds using analytical methods such as mass spectrometry for chemical contaminants<sup>50</sup> or polymerase chain reaction for viruses.<sup>38</sup> The known air flow rates of active samplers enable calculation of passive sampler uptake rates. Further details are provided on calibration



**Figure 5.** Wearable passive samplers collect a diverse range of gases, gas-phase chemicals, and particle-phase compounds from ambient air through diffusion and deposition. Contaminants move across stagnant boundary layers before reaching the sorbent. The mass of contaminants collected in this sorbent can be measured to assess personal exposure.



**Figure 6.** Wearable passive samplers collect chemicals from the air by diffusion across three phases. Contaminants are initially taken up in a linear phase that continues until the sampler has reached 25% of its capacity. This time is denoted as  $t_{25}$ . Accumulation of chemicals then continues in a curvi-linear phase until 95% of the sampler's uptake capacity has been reached. This time is denoted as  $t_{95}$ . Exposure assessment periods extending beyond this time then continue in the equilibrium phase.

studies in Question 3.1 and on factors that influence uptake profiles in Questions 4.1 - 4.5.

## Quantifying exposure concentrations

Before wearable passive samplers can be used to quantify concentrations (volumetric air concentration, *eg*,  $\text{ng}/\text{m}^3$ ), calibration is required to characterize contaminant uptake rates and determine the sampling time needed to reach equilibrium. The parameters obtained from calibration can then be applied in field studies to convert the mass of chemical collected by the sorbent

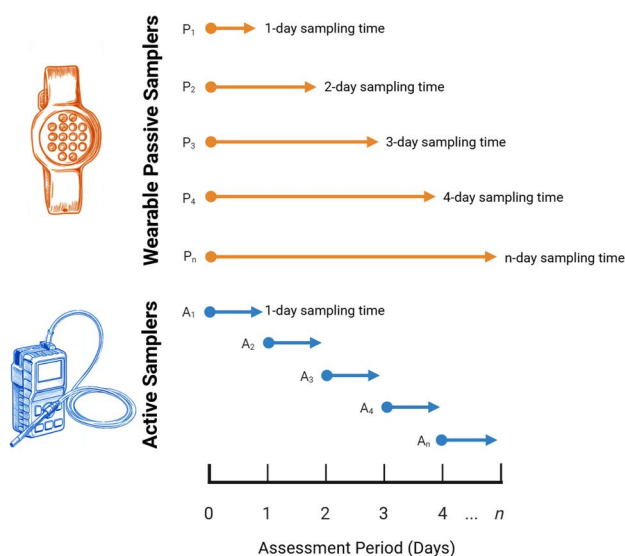
(chemical mass measured in nanogram) to a volumetric exposure concentration. The calibration protocols described in this section refer specifically to sampler designs that exclusively sample air (Fresh Air samplers, Brooch). For samplers that uptake contaminants from both air and skin (commercial silicone band, custom silicone band), modified protocols are required to include the uptake rate from dermal contact. This section describes how wearable passive samplers can be calibrated and used to estimate volumetric concentrations of compounds in the air.

### Question 3.1 How are wearable passive samplers calibrated?

As wearable passive air samplers do not contain a pump to actively move air, the mass of contaminants collected by the sampler cannot be directly converted to volumetric concentration (*ie*,  $\text{ng}/\text{m}^3$ ). To determine the volume of air passively sampled by these exposure assessment tools, calibration is needed against an active air sampler (*ie*, a device with a known volume of sampled air). Calibration can also guide how long a wearable passive sampler should be worn. The ideal sampling time will be within the linear phase of passive sampling to reflect the time-weighted average concentration of exposure. Sampling times can continue for longer with collection extended into the equilibrium phase. In this case, the sorbent-air partition ratio can be used to estimate the exposure concentration of measured contaminants at the time of sampler retrieval.<sup>13,51</sup>

Wearable passive samplers can be calibrated against an active sampler while being worn by a person or co-located at a stationary location in a controlled environment with relatively constant air concentration.<sup>43,52</sup> Another approach involves spiking deuration chemicals into passive samplers and correlating their loss rate to uptake rate,<sup>9,43,53</sup> but this is not encouraged since participants would be exposed to deuration chemicals. This section describes calibration of worn and stationary samplers against active air samplers.

When calibrating against an active sampler, both the wearable passive sampler and the active sampler must be simultaneously exposed to the same environmental contaminants and ideally collect compounds onto similar sorbent materials



**Figure 7.** Calibration of passive samplers against active air samplers in a hypothetical  $n$ -day exposure study. Blanks for both active and passive samplers should also be collected daily or at the start and end of the exposure period. Replicates for both active and passive samplers should be included as needed. Study duration should continue until the passive sampler has reached the equilibrium phase to calculate its equilibrium capacity ( $t_{25}$ ).

contained in a sorbent tube or filter cartridge. Calibration studies have used sorbent tubes with PUF and styrene divinylbenzene copolymer (PUF/XAD/PUF) sandwich (ORBO 49P (OVS) Supelpak, Sigma Aldrich) or PDMS foams (Gerstel).<sup>43</sup> Active and wearable passive samplers should be deployed over a range of sampling times that cover the linear to equilibrium phases of uptake (Figure 7). Blanks for both sampler types should be collected to monitor potential contaminations.

Multiple passive samplers are deployed, and one sampler is retrieved at each desired time point.<sup>43</sup> The wearable passive samplers are exposed for varying durations, whereas the active samplers are exposed for fixed durations (Figure 7). For a multi-day calibration study, all passive samplers are deployed at the start alongside an active air sampler. At the end of day 1, one passive air sampler is retrieved. The active sampler is also collected and replaced with a new sample. This process of periodically retrieving passive air samplers and replacing active samplers continues until all passive samplers have been retrieved.

Sampler placement is crucial when calibrating a sampler. For samplers that are worn during a calibration study, participants should wear passive and active samplers in approximately the same location. This strategy can be inconvenient or impractical for some sampler designs. For example, this would require wearing 10 brooches (including duplicates) and one active sampler simultaneously in the same location during a 5-day study.

It is often preferable or more practical to calibrate passive samplers in stationary locations to avoid the logistical challenges of wearing multiple wristbands or brooches over multiple days together with an active sampler. In this approach, wearable passive samplers (unworn) can be calibrated in an environment where experimental conditions are controlled to reflect the conditions of worn samplers.<sup>54</sup> For example, the samplers can be exposed to varying wind speeds to approximate changes in wind speed for a sampler worn during different personal activities (see Question 4.5 for details).

For particle or aerosol calibration, the rate of uptake or deposition is commonly determined in a rotating drum to keep contaminants suspended and control experimental conditions.<sup>32</sup> The protocol for deployment and retrieval is similar to the calibration for gases and gas-phase contaminants. In brief, the active sampler and passive sampler are deployed in an aluminum drum rotating at a constant speed. The drum is supplied with filtered air and generated aerosols, whilst aerosol concentrations are monitored in real-time. Collected samplers are often analyzed using gravimetric or analytical techniques, such as microscopy, spectroscopy, and/or elemental analysis, along with particle density and size distribution data. Together, these parameters allow for the calculation of deposition flux and mass transfer coefficient (also known as depositional velocity), which can then be used to estimate time-weighted average exposure concentrations for assessment periods.<sup>55</sup>

The described protocol for a calibration study may not apply to commercial silicone wristbands and custom silicone bands as they sample a combination of dermal and airborne contaminants. If wearable passive samplers capture multiple exposure pathways, it is not possible to convert measured contaminant mass loadings to air concentrations. It is important to understand the objectives of a study and select the appropriate assessment tool that will provide the desired exposure measures.

Measurements obtained from active and wearable passive samplers co-deployed over multiple time intervals can be used to generate an uptake curve (Table 1) where equivalent air volume (eqn (1)) is plotted against deployment time. The slope of the uptake curve, forced through the origin (assuming no background contamination), represents the uptake rate.<sup>12,13</sup> This rate can be established for individual compounds, and the representative statistic of multiple compounds can also be taken to derive a generic uptake rate for the wearable passive sampler when sampling for gas-phase chemicals.<sup>43</sup> The use of a generic uptake rate should ideally be limited to gas-phase chemicals only and is justifiable since the uptake rate should be theoretically similar for all gas-phase chemicals captured during linear sampling under similar conditions.<sup>13,40</sup> The decision to use generic uptake rates versus compound-specific rates should be weighed carefully when uptake rates vary beyond 20% relative standard deviation. Variability in uptake rates between individual chemicals and chemical classes assessed at the same location is likely attributable to varying concentrations and partition behaviors between the gas and particle phases.

$$\text{Equivalent air volume (m}^3\text{)} = \text{Uptake rate (Slope, m}^3\text{day}^{-1}\text{)} \times \text{Exposure assessment time (day)} \quad (1)$$

Calibration studies demonstrate how environmental conditions and activity patterns influence derived rates. For the brooch sampler in office environments, values ranged from 0.40 to 1.32 m<sup>3</sup>/day/dm<sup>2</sup> with a generic value of 0.86 ± 0.29 m<sup>3</sup>/day/dm<sup>2</sup>.<sup>43</sup> These values were derived using samplers for four phthalates and one organophosphate ester. In contrast, measurements among electronic waste workers, a generic rate of 19 ± 11 m<sup>3</sup>/day/dm<sup>2</sup> (range 5.7 to 40) was found. The rate was based on four brominated flame retardants and three organophosphate esters.<sup>23</sup> The higher values for waste workers compared to the office study was attributed to the dusty nature of the workplace and the increased effect of wind speed on the sampler due to worker movements. The wide range and standard deviation in the reported rates highlight the high variability in the degree of activity or movement amongst the workers.

**Table 1.** Parameters used to derive uptake curves during calibration of wearable passive samplers against active samplers.

Assessment period (days)	Passive samplers contaminant mass loading (ng)	Active sampler contaminant air concentration (ng/m <sup>3</sup> )	Equivalent air volume (m <sup>3</sup> )
t <sub>1</sub>	M <sub>1</sub>	C <sub>1</sub> *	M <sub>1</sub> /C <sub>1</sub> *
t <sub>2</sub>	M <sub>2</sub>	C <sub>2</sub> *=Average C <sub>(1&amp;2)</sub>	M <sub>2</sub> /C <sub>2</sub> *
t <sub>3</sub>	M <sub>3</sub>	C <sub>3</sub> *=Average C <sub>(1,2&amp;3)</sub>	M <sub>3</sub> /C <sub>3</sub> *
t <sub>4</sub>	M <sub>4</sub>	C <sub>4</sub> *=Average C <sub>(1,2,3&amp;4)</sub>	M <sub>4</sub> /C <sub>4</sub> *
t <sub>n</sub>	M <sub>n</sub>	C <sub>n</sub> *=Average C <sub>(1,2,3,4 ... n)</sub>	M <sub>n</sub> /C <sub>n</sub> *

Notes: Each sampler should be blank corrected based on laboratory criteria. For example, samples are not blank-corrected when chemical levels in blanks are less than 5% of sample levels, are corrected when blank levels are 6-35% of sample levels, and are discarded when blank levels exceed 35%.<sup>56</sup> Papers should also report whether measured chemicals were corrected based on surrogate standard recovery.

### Question 3.2 How can exposure concentrations be determined from wearable passive samplers?

A calibrated wearable passive sampler can be used to determine personal exposure concentrations. The ideal sampling duration is within the linear phase of uptake. The measured mass of contaminants collected by the wearable passive sampler during an assessment period can be converted to exposure concentrations using eqn (2).

$$\text{Concentration} \left( \frac{\text{ng}}{\text{m}^3} \right) = \frac{\text{Mass of chemicals captured (ng)}}{\text{Uptake rate} \left( \frac{\text{m}^3}{\text{day}} \right) \times \text{Assessment time (days)}} \quad (2)$$

For cases where the assessment period extends beyond the linear phase of uptake, exposure concentrations can be determined using eqn (3). This equation assumes that the sample was collected in the equilibrium phase and requires the sorbent-air partition ratio of the compounds of interest.

$$\text{Concentration} \left( \frac{\text{ng}}{\text{m}^3} \right) = \frac{\text{Mass of chemicals captured (ng)/sorbent volume (m}^3)}{\text{Sorbent - air partition ratio} \left( \frac{\text{m}^3 \text{ of sorbent}}{\text{m}^3 \text{ of air}} \right)} \quad (3)$$

When using wearable passive samplers to quantitatively measure exposure concentrations, it is recommended that assessment periods fall within the linear or equilibrium phases of sampling. The non-linear uptake rate in the curvi-linear phase presents challenges for calibration, so sampling in this phase should be avoided.

### Question 3.3 How long should a wearable passive sampler be worn to assess exposure?

Ideally, when designing a study that uses wearable passive samplers, the exposure assessment period should be limited to the duration within the linear phase of uptake. This duration depends on the capacity of the sampler's sorbent and can be determined through a calibration study or estimated. The measured sorbent-air partition ratio ( $K_{\text{sorbent-air}}$ ) and the sorbent volume<sup>13,51,56</sup> can be used to calculate the duration for linear sampling (eqn (4)).

$$\text{Exposure Assessment Duration for Linear Phase Sampling (days)} = -\ln(0.75) \left( \frac{\text{Sorbent Volume (m}^3) \times K_{\text{Sorbent-Air}} \left( \frac{\text{m}^3 \text{ of sorbent}}{\text{m}^3 \text{ of air}} \right)}{\text{Uptake Rate} \left( \frac{\text{m}^3}{\text{day}} \right)} \right) \quad (4)$$

Studies have examined how long wearable passive samplers can be worn while sampling compounds in the linear range. Figure 8 shows the linear uptake capacity of the brooch for 76

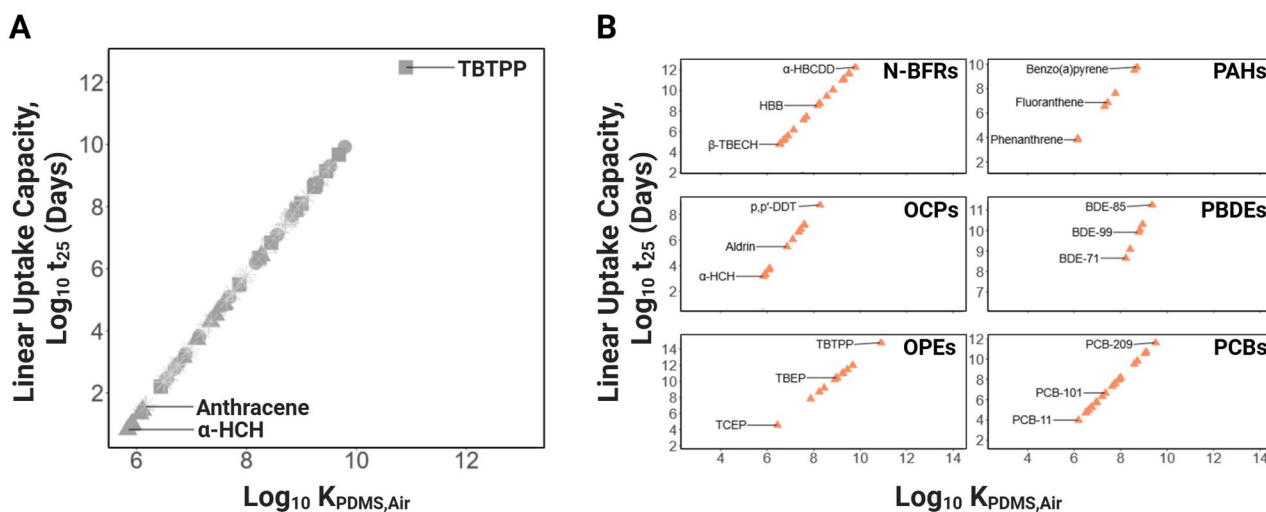
gas-phase chemicals with measured  $K_{\text{sorbent-air}}$  (ie,  $K_{\text{PDMS-air}}$ ) values.<sup>51</sup> The linear uptake capacity of this PDMS-based sampler ranged from two days for alpha hexachlorohexane ( $\alpha$ -HCH) to approximately 720 years for 4-tert-butylphenyl phosphate (TBTTP) when assessed at 25°C. The estimates cover a volatility range of 6 log units. These results suggest that if the brooch were worn for five days, compounds with log  $K_{\text{PDMS-Air}}$  values of less than or equal to 6.16 (eg, anthracene) would exceed the capacity of this wearable device in the linear sampling phase. Sampling beyond the linear phase requires using eqn (3) to estimate the exposure concentrations for chemicals with uptake that has reached the equilibrium phase. The estimated concentrations will be inaccurate if the chemical uptake is in the curvi-linear phase. Eqns (2) and (3) should be used as guides to ensure that concentrations are estimated when uptake is well within the linear or equilibrium uptake phases to avoid uncertainties in reported concentrations. Studies interested in capturing diverse compounds with varying lengths of linear uptake rates should combine Eqns (3) and (4) as some compounds will be in the linear phase while other compounds will be in the equilibrium phase.

### Question 3.4 When reporting exposure concentrations measured using wearable passive samplers, what information regarding the tool and calibration should be shared?

When describing exposure concentrations, the following calibration details of the wearable passive sampler should be provided: the environmental conditions under which the calibration was performed (temperature, humidity, wind speed), the uptake rate (eg, m<sup>3</sup>/day), the uptake rate normalized to the sampler's surface area (eg, m<sup>3</sup>/day/dm<sup>2</sup>), and the mass transfer coefficient (m/day). Uptake rates for individual compounds of interest as well as the generic uptake rate  $\pm$  standard deviation should also be reported. To improve reproducibility, studies using wearable passive samplers for personal exposure assessment should describe the device features or cite published papers that provide these details, including sorbent type and properties (eg, PDMS/silicone or other material), sorbent dimensions (length, width, thickness, volume, diameter, and circumference), and overall device dimensions excluding the sorbent (length, outer diameter, inner diameter, and area). When sheltered, the type and configuration of the sampler shelter (eg, stainless steel or Teflon/PTFE chamber) should also be reported. Where not proprietary, the suppliers of all materials (ie, sorbent, shelter, housing/support, etc.) should also be documented.

## Wearable passive sampler performance

The performance of wearable passive samplers is influenced by multiple factors ranging from the sampler design to ambient



**Figure 8.** Linear uptake capacity ( $t_{25}$ ) and log PDMS-air partition ratio ( $K_{\text{PDMS-air}}$ )<sup>51</sup> estimated for the brooch sampler using a generic uptake rate of  $0.43 \text{ m}^3/\text{day}$  (Okeme et al. 2016)<sup>51</sup> for (A). 72 chemicals and (B) Across six chemical classes.

conditions. This section describes the factors that influence the uptake rate and capacity of these wearable tools.

#### Question 4.1 What are factors that influence the rate and capacity of contaminant uptake by wearable passive samplers?

The rate of contaminant uptake by the sorbent of a wearable passive sampler can vary depending on parameters that impact diffusion or deposition, whether in a controlled environment or in the field. One major factor is how easily or quickly contaminants can cross the stagnant boundary layer surrounding the sampler. As described in Question 2.1, the rate is characterized by the mass transfer coefficient for gases as well as gas- and particle-phase chemicals, while the rate for particles collected is described by the deposition velocity.<sup>12,13,38</sup> Under controlled conditions (laboratory chamber), similar mass transfer coefficients for chemicals of different classes and varying volatilities have been reported for passive samplers with PDMS sorbents.<sup>57</sup> In the field, however, the uptake rates of various compounds differ across sorbents (eg, PDMS, XAD, and polyurethane foam).<sup>58</sup> This variability in the field can be explained by the type of sorbent material, configuration of the passive sampler (eg, sheltering), combined gas and particle sampling, chemical degradation or loss, site specific conditions (eg, temperature, wind speed, and humidity), and variability in ambient concentrations.<sup>12</sup> It is useful to note that all factors that influence uptake rate can also influence uptake capacity, including sorbent material, sampler design, chemical degradation or loss, site-specific conditions (wind speed, temperature, and humidity), and activity patterns. These factors are discussed in Question 5.2-5.7.

#### Question 4.2 How does the nature of sorbent and shelter of wearable passive sampler influence uptake of environmental contaminants?

Features that can influence the uptake of chemical contaminants include the sorbent material type and dimensions as well as the use of a housing case.

Uptake rates vary among sorbent materials due to their distinct surface structures or morphologies. For example, compared to PDMS, which is rubber-like, polyurethane foam is more efficient at collecting particles because of its large cavities.<sup>59</sup> Humidity can influence the uptake rates of certain sorbent

materials (eg, polyurethane foam and XAD) that absorb water.<sup>60</sup> In terms of dimensions, uptake rates increase with the exposed surface area of the sorbent material.

All four designs of common wearable passive samplers (commercial silicone wristbands, custom silicone bands, the brooch, and the Fresh Air samplers) use PDMS as the sorbent.<sup>9</sup> PDMS is an attractive sorbent for passive sampling because of its high permeability to many chemicals, versatility in that it can be designed into different shapes and sizes, ease of cleaning with less background contamination, chemical inertness and stability of sampling properties over a wide range of ambient conditions, well-characterized sorption properties, and high sorptive capacity.<sup>39,58</sup> Other sampling materials (eg, polyurethane foam, XAD) lack most, if not all, of these properties.

Stationary (non-wearable) passive samplers used outdoors shelter the sorbent to protect the material from precipitation, direct sunlight, and large debris.<sup>12,61,62</sup> Shelters are also used to reduce wind speed over the sorbent to minimize variability in uptake rate, as wind alters the thickness of the stagnant boundary layer over the sorbent (described in Question 3.1).<sup>63</sup> For the same reason, some wearable passive samplers shelter the sorbent (eg, Fresh Air samplers).

#### Question 4.3 What is the stability of chemicals collected by wearable passive samplers?

Chemicals can be susceptible to degradation once taken up by the sorbent,<sup>64</sup> but this is likely not a major concern for the short exposure assessment periods (less than 7 days) that are evaluated using wearable passive samplers. While degradation studies have not been conducted for PDMS sorbent used in wearable passive samplers, findings from stationary passive samplers with polyurethane foams suggest that degradation occurs after a month-long sampling period outdoors.<sup>64</sup> Specifically, researchers found higher mass loadings of PAHs measured in samplers that were collected weekly versus monthly. The difference between weekly and monthly samplers was more pronounced for chemicals that were more reactive (eg, benzo[a]pyrene) and less volatile, suggesting that loss was attributable to degradation rather than volatilization or reverse diffusion. Extended sampling periods (months) were estimated to introduce uncertainty of up to 4-fold for polyurethane foam passive samplers deployed outdoors.<sup>64</sup> Therefore, assessment of personal exposure using

wearable passive samplers over one to two weeks is recommended especially when it is of interest to assess more reactive compounds. This duration captures exposures from a range of weekday and weekend activities, maintains optimal participant compliance (remembering to wear the device daily), and avoids potential compound degradation.

In addition to degradation, more volatile chemicals collected by the sorbent are susceptible to losses by volatilization during wearable passive sampler retrieval, transport, storage and processing.<sup>12</sup> For example, in one study, over 50% of spiked labelled naphthalene and 1-methylnaphthalene were lost from the Fresh Air sorbent bars - after 24h when stored at room temperature compared with cold storage.<sup>11</sup> Another study assessed the stability of VOCs (eg, toluene and trichloroethylene) in the Waterloo Membrane Sampler, a permeation sampler, comprising a PDMS membrane and a receiving charcoal sorbent, both placed in an autosampler vial.<sup>48</sup> After three weeks storage at room temperature, the PDMS membrane only retained negligible amounts of the VOCs, whereas the chemicals were fully stable in the charcoal. Following the exposure assessment period, care should be taken to minimize losses by storing wearable passive sampler in air-tight containers at temperature-controlled conditions. Cold chain shipping is recommended when transporting samplers, and cold storage should be maintained prior to analysis. Transport and storage temperature controls and durations should be detailed when describing exposure findings.

#### **Question 4.4 What ambient factors impact the uptake of contaminants by wearable passive samplers?**

Uptake of contaminants by passive samplers is influenced by ambient conditions, including geography, temperature, humidity, and wind.<sup>12,52,58,65</sup> Of these factors, only wind speed has been strongly correlated with uptake rate ( $r^2 = 0.910$ ) in the field.<sup>66</sup> Variability in chemical concentrations within and between exposure assessment locations, notably indoor versus outdoor sites,<sup>52,61</sup> can also affect the uptake rate of compounds.<sup>56</sup> Alternating between indoors and outdoors has been suggested to alter the uptake kinetics by up to 10-fold,<sup>58</sup> since sampler uptake rates can be influenced by wind speed and differences in concentrations indoors/outdoors due to proximity to exposure sources. To minimize the impact of these parameters, wearable passive samplers should be calibrated under similar conditions to those under which exposure will be assessed, especially for sampler designs that do not shelter the sorbent.

#### **Question 4.5 How does a person's activity patterns influence the uptake rate of wearable passive sampler?**

Activities with different levels of intensity (eg, running, walking, and arm movement) can change air movement over wearable passive samplers, which influences the uptake rate of contaminants. For example, wrist movements when walking can result in wind speeds of 0.05 to 1.1 m/s by the wrist. These movements translate to a  $1.2 \pm 0.2$  to  $4.3 \pm 0.8$  fold increase in uptake rate relative to a passive sampler deployed at a fixed location.<sup>54</sup> However, the effect of personal movement on the uptake rate of wearable passive samplers can be minimized by appropriate sampler design. Samplers with housing cases, such as those used in Fresh Air samplers, can reduce this variability.

In addition to movement-related factors, it is important that wearable passive samplers be worn in a manner that maximizes collection of contaminants from a range of sources. For

wristband-style samplers or the brooch, long-sleeved clothing or outer garments can interfere with chemical uptake by covering or blocking the samplers from ambient air, particularly during winter months.

To account for these various factors, samplers should be calibrated using a similar group of study participants or under simulated chamber conditions to reflect real-life usage, including the relative movement intensity, age, and lifestyle of study participants. In addition to movement-related factors, it is important that wearable passive samplers be worn in a manner that maximizes collection of contaminants from a range of sources. For wristband-style samplers or the brooch, long-sleeved clothing or outer garments can interfere with chemical uptake by covering or blocking the samplers from ambient air, particularly during winter months (See Question 6.1 for best practices on wristband wear). Understanding the performance of wearable passive samplers under different conditions that impact the boundary layer over the sorbent is essential to avoid over- or underestimated exposure estimates.

### **Sample preparation and chemical analysis**

Proper sample preparation and analytical methods are fundamental to obtaining reliable exposure data from wearable passive samplers. This section provides guidance on essential pre-deployment cleaning procedures, post-exposure sample handling, and analytical approaches for comprehensive chemical characterization. We address key decisions regarding extraction methods, analytical platforms, and data interpretation strategies.

#### **Question 5.1 How are wearable passive samplers prepared for use to assess environmental exposures?**

All wearable passive samplers require cleaning before use. Cleaning involves using solvent or solventless methods to remove background contaminants from sorbents and other sampling materials (such as housing materials).<sup>9</sup> Solvent cleaning typically involves flushing the sampling material with solvent using apparatus such as a Soxhlet extractor or an accelerated solvent extractor.<sup>67</sup> Solventless methods involve heating the sampling material in a vacuum oven.<sup>68</sup> It is not sufficient to clean wearable samplers with water and soap as this process will not effectively remove background contaminants and may introduce further contamination.

Prior to deployment, cleaned wearable passive sampler should be stored in air-tight clean containers that are composed of inert materials that will not introduce contamination (eg, glass).<sup>69</sup> Containers should be tested for background contamination over time periods that reflect typical storage durations.

Following the exposure assessment period but prior to instrumental analysis, some sample preparation methods involve rinsing the sorbent material in the wearable passive sampler with deionized water. While this rinsing step is used in protocols to remove dust and larger debris, this clean-up step can potentially remove chemicals of interest through dissolution of polar chemicals. If washing is necessary, chemical losses should be assessed by comparing recoveries of methods with and without washing. Contaminants collected by the sorbent in the wearable passive sampler can be extracted using solvents or heat (thermal desorption).<sup>11,23,44</sup>

It is important to describe the methods used for cleaning, storing, and extracting wearable passive samplers when reporting exposures. As a minimum, the cleaning protocol should report

solvent type(s), sampler cleaning apparatus (eg, Soxhlet, vacuum oven), conditions (eg, temperature, nitrogen flow), and duration. Storage containers (materials, cleaning protocols) should also be described.

### Question 5.2 What analytical techniques can be used to assess environmental contaminants collected by wearable passive samplers?

Chemicals extracted from wearable passive samplers can be assessed using any technique that can analyse contaminants collected by the sorbent either directly or after extraction. Selecting a technique is ultimately guided by the range of contaminants of interest. Chemical analysis of wearable passive samplers has typically been conducted using mass spectrometry, and biological analysis has been performed using sequencing techniques. Mass spectrometry can be used to analyse trace metals (using inductively coupled plasma mass spectrometry, ICP-MS)<sup>70</sup> and organic compounds (using gas chromatography mass spectrometry, GC-MS, and liquid chromatography mass spectrometry, LC-MS). Polymerase chain reaction (PCR) can be used for detecting viruses, including SARS-CoV-2<sup>38</sup> as well as pollen and bacterial contaminants.<sup>71</sup> In addition to chemical and biological analyses, physical characteristics of contaminants collected on wearable passive samplers can be assessed using colorimetric and other light-based techniques, such as optical microscopy and scanning electron microscopy.<sup>49</sup>

### Question 5.3 What mass spectrometry approaches can be used to comprehensively measure organic chemical contaminants collected by wearable passive samplers?

Mass spectrometry offers the most comprehensive and sensitive measurement approach for analysing chemical contaminants collected using wearable passive samplers. Mass spectrometry can be coupled with different separation techniques, including liquid chromatography, gas chromatography, and ion mobility,<sup>72</sup> which provide complementary coverage based on compound amenability to each technique.<sup>73</sup> Mass spectrometry analysis can be conducted using targeted, suspect screening, and non-targeted approaches (see Question 5.4). Mass spectrometers used for chemical detection and characterization of wearable passive samplers include single quadrupole, triple quadrupole, quadrupole time-of-flight, and quadrupole Orbitrap mass spectrometers.<sup>9,11,23,74-76</sup>

While gas chromatography and liquid chromatography are complementary approaches, the former approach has been used in about 90% of wearable passive sampling studies.<sup>9</sup> Liquid chromatography has been applied in select studies using commercial wristbands<sup>77-91</sup> Gas chromatography covers more volatile and semi-volatile molecules (often lower molecular weight and more nonpolar compounds) than liquid chromatography. Liquid chromatography covers a wider range of higher molecular weight and polar molecules than gas chromatography.<sup>4</sup> Hence these two methods are highly complementary, together covering a wider range of polarities and molecular weights. Gas chromatography has additional advantages including the ability to directly measure analytes from wearable passive samplers, simplified retention index calculation for confident annotation, and harmonized acquisition methods and libraries of over 1 million analyte spectra (mainly low resolution) deploying these harmonized methods.<sup>74</sup> GC-MS spectral libraries have not scaled with the advent of high-resolution mass spectrometry; high-resolution spectral matching drastically reduces the false positive rate in targeted,

non-targeted, and suspect screening methods. Only a small fraction of the major GC-MS libraries (eg, NIST/WILEY libraries) are high-resolution, whereas a significant portion of LC-MS/MS libraries, both commercial (eg, mzCloud, NIST, and Wiley) and open-source (eg, HMDB, MassBank, and GNPS) are now high-resolution (tens of thousands of molecules, millions of spectra), signifying more community support. Additionally, ions have similar ionization efficiencies in gas chromatography irrespective of structure, making quantitation in non-targeted analyses easier than in liquid chromatography where ionization efficiencies are affected by chemical structure. One disadvantage of gas chromatography, especially when using electron impact (EI) ionization, is that the molecular ion often cannot be determined readily and similar spectra across isomers leads to difficulties determining subtle isomeric differences.

Ion mobility theoretically could be placed after both gas and liquid chromatography, although in practice ion mobility has been used mainly with liquid chromatography. Ion mobility provides an additional separation dimension which can be deployed alongside liquid chromatography for better specificity (increasing coverage of isomers) and collision cross section values provided by ion mobility can be used as an additional important piece of evidence for chemical identification reducing false positives.<sup>92</sup> It can also be used without other separation techniques to perform rapid separation (seconds versus minutes to hours), reducing analysis time and costs whilst being more reproducible. However, ion mobility has much lower resolving power in most cases compared to liquid chromatography and gas chromatography, meaning fewer molecules can be separated. Furthermore, for ion mobility sensitivity will be reduced due to ion suppression issues at the source (all ions competing for ionization simultaneously, rather than being separated out in time when liquid chromatography is used). Ion suppression when using ion mobility separation without liquid chromatography is a major issue because mobility separation occurs *after* the ionization source, leading to the entire sample being introduced onto the mass spectrometer at once (more molecules competing for ionization). Currently there is no research applying ion mobility for personal exposure monitoring using passive samplers, although implementation of this approach would be trivial (exact same passive sampler preparation and extraction methods as used by LC-HRMS or GC-HRMS, but applying ion mobility acquisition and data-processing workflows which have already been developed for other applications). Application of ion mobility to analyze wearable passive sampler could reveal novel important exposures (previously unresolved isomers) and increase the throughput of identification and screening for chemicals of interest.

As mentioned, all configurations of chromatographic techniques combined with different mass spectrometry configurations discussed in this paper have been used to characterize wearable passive samples.<sup>9,11,23,74-76</sup> For mass spectrometry configurations, triple quadrupoles are generally used for targeted analysis and can be more sensitive detectors (higher ion transmission). Quadrupole time-of-flight and Orbitrap instruments offer higher mass resolution and accuracy and are therefore better suited for suspect screening and non-targeted approaches due to their higher specificity. These high-resolution mass spectrometers can further provide higher specificity in certain cases, reducing the potential for additive effects from matrix during quantitation and even lead to better sensitivity in certain cases.<sup>93-95</sup> Further details on methodologies and standard operating procedures for mass spectrometry can be found elsewhere.<sup>75,96-99</sup>

### Question 5.4 What are targeted, suspect screening, and non-targeted approaches for chemical analysis of wearable passive samplers?

Mass spectrometry analysis of wearable passive samplers can be conducted using three distinct analytical strategies, each with different capabilities and requirements depending on the study objectives and prior knowledge of expected contaminants.

*Non-targeted analysis* of wearable passive samplers can be used to discover unknown chemicals, providing the greatest chemical coverage. Non-targeted approaches are diverse but incorporate universal principles and class/structurally based patterns (in fragmentation, retention time, and/or exact mass) to either group compounds by class or structural patterns, or to assign structure.<sup>100-103</sup> This approach consists of several and often time-consuming steps, and results must always be manually validated. Non-targeted methods include homologous series detection,<sup>104</sup> molecular networks using spectral similarity,<sup>105</sup> machine learning algorithms for spectral and retention time prediction,<sup>106</sup> class-based fragment assignment,<sup>107</sup> and rule-based approaches for fragmentation assignment.<sup>107,108</sup>

*Suspect screening analysis*, a subcategory of non-targeted analysis,<sup>109</sup> can also be used to semi-quantitatively assess exposure to known chemical compounds. Rather than requiring authenticated standards for each compound, this technique takes advantage of community-wide mass spectral and/or retention index (or collision cross-section in the case of ion mobility) libraries that have been generated using authenticated standards.<sup>74</sup> These libraries also contain compound characteristics generated using predictive models, which can supplement standard information and standardize metrics irrespective of methodological differences (eg, retention index prediction).<sup>110</sup> Community-based libraries used for suspect screening analysis often contain hundreds of thousands (liquid chromatography) to over one million (gas chromatography) spectra, enabling more comprehensive exposure assessment compared to targeted methods.<sup>111</sup> Analysis of wearable passive samplers using this approach enables more comprehensive coverage with identification of potentially unexpected exposures not included in targeted chemical panels. For example, one study exploring personal exposures in older adults residing in an urban area in China using suspect screening analysis of Fresh Air wristbands detected dichlorvos exposures. This chemical was historically used for mosquito control, but its use has been banned in the United States as it is a neurotoxin. Despite not being included in a targeted exposure panel, suspect screening analysis identified exposure. The semi-quantitative nature of the analysis further revealed variance in levels across participants and seasons (30-fold increase in warmer months).<sup>3</sup> Suspect screening has some caveats. Use of unstandardized reference spectra and retention libraries generated by different laboratories using varying extraction methods, instruments, acquisition parameters, and data-processing workflows decreases the confidence of identified chemicals compared to targeted analysis and reduces the repeatability and reproducibility of exposure identification and abundance measurements. Comparison of exposures detected by suspect screening between laboratories requires confirmation by manual review and often purchase/synthesis of chemical standards using targeted analysis.<sup>74,111</sup>

*Targeted approaches* are used to quantify absolute masses or concentrations of a known panel of chemicals, unlike peak areas generated in nontargeted analysis. This type of analysis requires authenticated standards for all chemicals of interest. These standards are used to confidently identify measured chemicals

and quantify exposure levels quantitatively measure exposure levels using external or internal calibration curves.<sup>112</sup>

### Question 5.5 What type of exposure information can wearable passive samplers provide?

Wearable passive samplers can provide both quantitative, semi-quantitative, and qualitative exposure information. For *quantitative* assessment, exposure concentrations can be obtained from calibrated wearable passive samplers by applying uptake rates (see Question 3.1-3.2). Semi-quantitative applications are also possible when samplers are uncalibrated but analytical standards are available for the compounds of interest. In these cases, the mass of contaminants measured in the sorbent can be used to assess relative differences between exposure groups or study participants.

*Semi-quantitative* measurements can be further obtained in cases where authenticated standards are not available, such as when using suspect screening approaches. In these cases, chromatographic peak areas can be compared to assess variabilities or trends in exposure levels within and between different studies, populations, time periods, or geographical locations without requiring full calibration studies, though the absence of authenticated standards limits the ability to provide absolute concentration measurements.

For *qualitative* assessment, uncalibrated wearable passive samplers can be used to determine the presence or absence of contaminants, where the detection of an identified chemical is sufficient to establish its presence. This approach is valuable for exposure screening studies and non-targeted analysis where the goal is to identify previously unknown or unexpected chemical exposures.

### Question 5.6 Are exposures estimated using wearable passive samplers comparable to biological monitoring?

The relationship between chemical exposures measured using wearable passive samplers and biological markers of exposure has shown mixed results across studies.<sup>22,76,81,113,114</sup> These findings reflect the inherent challenges in comparing external exposure measurements with internal biomarkers, particularly given the different exposure pathways, temporal dynamics, and metabolic processes involved.

Evidence for variable correlations has been reported between exposures assessed using wearable passive samplers and biological samples, with results varying by chemical class and sampling duration.<sup>22,76,81,113,114</sup> Urine markers for PAHs,<sup>114</sup> OPEs,<sup>115</sup> phthalates,<sup>114</sup> and phenols<sup>81</sup> measured using commercial silicone wristbands worn for 2-7 consecutive days showed significant correlations with their corresponding exposure markers in urine ( $P < 0.05$ ). Separately, BDE-209 levels in custom silicone wristbands worn for eight hours showed moderate correlations with plasma concentrations ( $r_s = 0.40$ ,  $P < 0.05$ ).<sup>23</sup> However, several studies have reported weak or no correlations for other chemical classes and sampling conditions. OPEs measured using custom silicone wristbands, worn for eight hours, were not correlated with levels of OPE metabolites in paired spot urine samples ( $r_s = 0.08$  to  $0.34$ ,  $P = 0.08$  to  $0.97$ ).<sup>23</sup> The difference in OPE correlations between wristband designs may be attributable to the longer wearing duration (5 days versus eight hours) and the use of pooled versus single spot urine samples.<sup>76</sup>

Several factors contribute to the variability in correlations between wearable passive samplers and biological markers of exposure. Assessment duration is critical, with longer sampling periods showing improved agreement with biomarkers.<sup>23</sup> Different exposure pathways also contribute to variability, as biological samples (plasma and urine) integrate exposure from

inhalation, dermal, and ingestion pathways, whilst some samplers only assess airborne exposure. The pharmacokinetic properties of specific chemicals, including their biological half-lives, play a crucial role in determining correlation strength—for example, OPEs showed weak correlations likely due to their short half-life ranging from hours to days.<sup>115-117</sup>

## Framework for harmonization

Successful implementation of wearable passive samplers in exposome research requires adherence to a comprehensive framework of standardized practices throughout the entire study workflow. This section consolidates essential guidelines for ensuring data reproducibility and harmonization across studies, from sample collection through analytical measurement and data reporting. We present minimum standards and recommended protocols that enable meaningful comparison of exposure findings between research groups and facilitate secondary analysis of existing literature. These standardized approaches are critical for advancing the field toward routine use in large-scale health studies and regulatory applications where data transparency and cross-study comparability are essential.

### Question 6.1 What best practices ensure reliable and reproducible results from wearable passive sampler studies?

The recommended practices outlined below draw from extensive experience developing, validating, and applying wearable passive sampler technologies over the past decade. This work has encompassed initial technology development, comprehensive validation studies comparing performance against traditional exposure assessment methods, and subsequent implementation in large-scale epidemiological investigations. These practices address critical control points that, when properly managed, ensure robust and defensible exposure data suitable for regulatory and research applications.

#### Sample collection

##### Sampler design

Document the rationale for wearable passive sampler selection based on study objectives, clearly stating the desired exposure measures (eg, airborne concentrations, qualitative screening) that informed hardware selection. Report key design specifications including sorbent type and dimensions, housing configuration (if applicable), and supplier information. Specify the source of captured contaminants—air, skin, or both—as this distinction determines the type of exposure data that can be generated and must align with the study's exposure assessment goals.

##### Exposure assessment duration

Ensure that samplers are deployed within their validated linear uptake phase to obtain quantitative or semi-quantitative exposure estimates and document the linear sampling duration limits established during calibration. Limit the sampling period to one to two weeks maximum to reduce the potential for sample degradation if it is of interest to assess of more reactive compounds. However, if the goal is to assess less volatile, highly persistent organic compounds (eg, PFAS or high molecular weight brominated flame retardants), a longer sampling duration—beyond two weeks—may be necessary to achieve a sufficient limit of detection.

##### Instruction on wear

Provide participants with written instructions and visual aids demonstrating proper sampler placement and care. Instruct

participants to keep their wearable passive sampler properly exposed to ambient air throughout the assessment period (eg, not covered by clothing for extended periods), and avoid applying personal care products directly to the samplers (eg, lotion, perfume). Participants should also refrain from wearing the device during water immersion activities (eg, showering, bathing, swimming, washing), unless the study aims to assess exposure to contaminants arising from these activities.

##### Calibration parameters

For calibrated samplers, report the uptake rate(s) used for volumetric concentration calculations, environmental conditions under which calibration was performed, and whether compound-specific or generic uptake rates were applied.

##### Cleaning and storage protocols

All wearable passive samplers must undergo thorough pre-deployment cleaning using appropriate solvent or solventless methods to remove background contaminants from sorbents and housing materials. Document cleaning protocols including solvent types, methods, conditions, and duration. Store cleaned samplers in air-tight containers composed of inert materials that have been tested for background contamination over typical storage periods. Following exposure assessment, maintain cold-chain storage in sealed, contaminant-free containers.

##### Background contamination control

Chemicals of interest should originate from exposure sources, not from background contamination introduced during sample handling or transport. Two types of blanks are essential for monitoring contamination:

- Laboratory blanks are unexposed samplers that undergo cleaning, storage, and analytical procedures but are never deployed in the field. These control for contamination from laboratory processes, storage materials, and analytical procedures.
- Field blanks accompany exposure samples through all field deployment procedures (transport, handling, storage conditions) but are never worn by participants. These blanks should be analyzed to account for potential field-related contamination and enable measurement adjustment.<sup>118</sup>

##### Management of batch effects

When assessing exposure dynamics (eg, changes across seasons or geographical locations), samples should be treated as equally as possible. This includes random assignment in run order and across batches, consistent collection and transport procedures, standardized storage conditions and durations, and identical acquisition methods. Include quality control samples distributed throughout analytical batches. Any differences in sample handling must be clearly documented, and their impact demonstrated to be negligible compared to exposure-related changes.

##### Sample processing Sample degradation

Monitor for chemical degradation during transport, storage, and processing, particularly for reactive compounds. Use cold-temperature transport and storage (<4°C when possible) to limit the potential for sample degradation. Document storage temperatures and durations throughout the sample handling process.

### Extraction efficiency

Recovery should be determined and clearly reported based on surrogate standards spiked into samples before extraction. Surrogate standards are analogues or isotopes of chemicals of interest that do not exist naturally in the environment. Report recovery rates for individual surrogate standards and apply recovery corrections to measured concentrations where appropriate.

### Preventing cross-contamination

Use separate equipment for different samples and follow established cleaning protocols between samples to prevent cross-contamination during sample cleaning, extraction, and processing. Process samples in randomized order and include procedural blanks to monitor for cross-contamination between sample batches. Use analytical standards to assess cross-contamination throughout sample processing.

### Sample measurement

#### Analytical approach specification

Specify the analytical approach employed (targeted, suspect screening, or non-targeted) as this determines the type of exposure data generated. Targeted analyses using authenticated standards enable high-confidence quantitative exposure concentrations, suspect screening provides semi-quantitative estimates with moderate confidence, while non-targeted approaches yield qualitative exposure profiles for chemical discovery.

#### Calibration standards

For targeted analysis, standard calibration curves must cover the expected concentration range found in wearable samples. These curves should be constructed using authenticated standards that produce response factors within 20%. Response factors are calculated differently depending on the calibration method employed. In internal calibration, the response factor is the ratio of analyte signal to internal standard signal. In external calibration, the response factor represents the instrument's response relative to known standard concentrations.

#### Matrix effects assessment

Evaluate and account for matrix effects that could influence ionization efficiency. Assess matrix effects using post-extraction spiked samples or standard addition methods and apply appropriate corrections when matrix suppression or enhancement exceeds reasonable limits (typically  $\pm 20\%$ ).

#### Data processing quality control

Apply blank feature filtering<sup>119</sup> or other techniques to remove signals below established thresholds (equivalent to the limit of quantification) that are not from personal exposure.

#### False positive identification

For suspect screening and non-targeted analyses, establish criteria for confidence in structural assignment and clearly communicate metrics used for annotation following accepted community protocols.<sup>74,104,120-123</sup> For suspect screening analysis, report the criteria used to assign confidence levels to annotated chemicals, confidence levels for all annotated compounds, and include supporting evidence such as retention time matching, mass accuracy, and fragmentation patterns.

#### Precision and accuracy

Assess precision through replicate sample analysis and accuracy through standard reference materials and inter-laboratory

comparisons (when applicable) when more than one laboratory is involved. Report coefficients of variation for precision studies and percent recovery for accuracy assessments.

### Analytical performance reporting

Clearly report analytical performance parameters for targeted analyses, including detection limits, and any applied blank correction procedures.

### Instrument performance

Control and report batch effects, instrument drift and other run-order effects, carry-over, and other technical factors that could influence measured chemical abundances. Implement regular quality control sample analysis throughout analytical runs and document any corrective actions taken.

### Exposure reporting units

Report exposure data using appropriate units based on sampler design, calibration status, and analytical approach. Volumetric exposure concentrations ( $\text{ng}/\text{m}^3$ ) can only be calculated for targeted analysis of calibrated samplers that exclusively sample air. For targeted analysis of uncalibrated samplers, exposures should be reported as mass loadings (eg, mass of chemical per mass of silicone). Clearly state measurement units and analytical confidence levels to ensure appropriate data interpretation.

Additional details regarding standardized practices for environmental exposure assessment have been previously described.<sup>3,74,98,124,125</sup> Comprehensive documentation of all implemented procedures in publications is essential to ensure study reproducibility and enable meaningful comparison of exposure data across different research groups and studies. The applicability and impact of wearable passive sampler technologies will continue to grow as these standardized methods are further developed and validated.

## Conclusions

Wearable passive samplers are minimally invasive tools with enormous potential for advancing personal exposure assessment. Rapid advancement of this technology over the past decade has operationalized measurement of the chemical and biological features of an individual's exposome, leading to widespread adoption across diverse study populations. The simplicity of this tool allows for straightforward integration into prospective large-scale studies of human disease, where samples can be easily collected and banked, capturing environmental information for future analysis as new research questions emerge and analytical capabilities advance. However, without consistent methodological approaches, the full potential for cross-study comparison and data harmonization cannot be realized. This review has addressed critical questions covering all aspects of designing, calibrating, and applying wearable passive samplers in research studies. Successful implementation requires matching sampler design to study objectives—distinguishing between the exposure metrics provided by wearables that exclusively capture airborne contaminants versus those that integrate multiple exposure pathways—and understanding the fundamental principles of passive sampling and analytical methods. This includes calibration requirements to determine optimal wearing duration and measurement method selection based on desired data confidence levels.

The presented framework aims to support harmonization of wearable passive sampler language, sample collection protocols,

and high-throughput analysis methods to improve data transparency and the comparability of results between laboratories and studies. By providing systematic methods to longitudinally assess individual-level exposures, these tools can further be integrated with other omics technologies and geospatial data to address critical gaps in understanding human health and disease. This integrated approach will enable population-scale analysis that supports evidence-based policy development and implementation of targeted exposure reduction interventions.

## Author contributions

Joseph Okeme (Conceptualization [equal], Formal analysis [equal], Funding acquisition [equal], Visualization [equal], Writing—original draft [equal], Writing—review & editing [equal]), Elizabeth Z. Lin (Conceptualization [equal], Formal analysis [equal], Writing—original draft [equal], Writing—review & editing [equal]), Jeremy P. Koelmel (Formal analysis [equal], Writing—original draft [equal], Writing—review & editing [equal]), Anya Guo (Writing—original draft [equal]), and Dong Gao (Writing—original draft [equal], Writing—review & editing [equal]), Krystal Pollitt (Conceptualization [equal], Funding acquisition [equal], Supervision [equal], Visualization [equal], Writing—original draft [equal], Writing—review & editing [equal])

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Dr. Krystal J. Godri Pollitt holds the position of Associate Editor for *Exposome* and has not peer reviewed or made any editorial decisions for this article.

## Conflict of interest

None declared.

## Data Availability

The data underlying this article will be shared on reasonable request to the corresponding author.

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