This article contains data on experimental sorption isotherms of 21 probe sorbates by aged polystyrene microplastics. The polymeric particles were subjected to an UV-induced photo-oxidation procedure using hydrogen peroxide in a custom-made aging chamber. Sorption data were obtained for aged particles. The experimental sorption data was modelled using both single- and poly-parameter linear free-energy relationships. For discussion and interpretation of the presented data, refer to the research article entitled “Sorption of organic compounds by aged polystyrene microplastic particles” (Hüffer et al., 2018) [1].

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**Value of the data**

- Sorption isotherm data for UV-aged polystyrene microplastic were determined for 21 molecular probe sorbates covering a broad spectrum of molecular substance classes.
- Modelling data provided information for the interpretation of molecular interactions between UV-aged polystyrene microplastics and organic compounds.
- Modelling data are valuable for the prediction of sorption by UV-aged polystyrene microplastics and allow a comparison with data from other aging processes and environmentally relevant polymers particles.

1. **Data**

Physico-chemical properties of the probe sorbates are given in Table 1. Fig. 1 shows sorption kinetics data of naphthalene by aged polystyrene microplastics (PSMP). Freundlich model fit data from sorption isotherms are shown in Table 2. A comparison of Freundlich fit model data between pristine and UV-aged polystyrene microplastics is given in Table 3. Data from statistical analyses of poly-parameter linear free-energy relationship model are shown in Tables 4–7.

### Table 1

| Compound          | log $S_w^b$ | log $K_{aw}^c$ | log $K_{ow}^d$ | E   | S   | A   | B   | V    | L    |
|-------------------|-------------|----------------|----------------|-----|-----|-----|-----|------|------|
| n-Hexane (nHex)   | 0.98        | 1.73           | 3.90           | 0.00 | 0.00 | 0.00 | 0.00 | 0.954 | 2.688 |
| Isohexane (iHex)  | 1.15        | 1.75           | 3.21           | 0.00 | 0.00 | 0.00 | 0.00 | 0.954 | 2.503 |
| Cyclohexane (cHex)| 1.74        | 0.78           | 3.44           | 0.31 | 0.10 | 0.00 | 0.00 | 0.845 | 2.964 |
| Dichloromethane (DCM)| 4.11      | 1.15           | 0.39           | 0.57 | 0.10 | 0.05 | 0.494| 2.019 |
| Tetrachloromethane (TCE)| 2.90   | −0.02          | 2.83           | 0.46 | 0.38 | 0.00 | 0.00 | 0.739 | 2.823 |
| Di-n-propyl ether (DPE)| 3.69  | −0.97          | 2.03           | 0.01 | 0.22 | 0.00 | 0.45 | 1.013 | 2.803 |
| 2-octanone (2ON)  | 2.95        | −1.98          | 2.37           | 0.11 | 0.68 | 0.00 | 0.51 | 1.252 | 4.257 |
| Hexanenitrile (HNT)| 3.39        | −2.30          | 1.66           | 0.17 | 0.90 | 0.00 | 0.36 | 0.968 | 3.513 |
| 1-nitrohexane (1NH)| 2.26        | 0.20           | 0.95           | 0.00 | 0.29 | 1.128| 4.416|
| 2-octanol (2OL)   | 3.05        | 0.16           | 0.36           | 0.33 | 0.56 | 1.295| 4.339|
| 3-ethylhexanol-3 (3EH)| 3.17 | 0.20           | 0.30           | 0.31 | 0.64 | 1.154| 3.805|
| 2,6-dimethylheptanol-2 (DMH)| 2.76 | −2.30  | 0.13           | 0.27 | 0.31 | 0.60 | 1.435| 4.469|
| Benzene (BEZ)     | 3.25        | 0.65           | 2.17           | 0.61 | 0.52 | 0.00 | 0.14 | 0.716 | 2.786 |
| Toluene (TOL)     | 2.72        | −0.60          | 2.69           | 0.60 | 0.52 | 0.00 | 0.14 | 0.857 | 3.325 |
| Chlorobenzene (CBZ)| 2.70        | −0.80          | 2.84           | 0.72 | 0.65 | 0.00 | 0.07 | 0.839 | 4.230 |
| Naphthalene (NAP) | 1.49        | 3.30           | 1.34           | 0.92 | 0.00 | 0.20 | 1.085| 5.161 |
| Benzothiazole (BTZ)| 3.63        | 1.37           | 0.65           | 0.36 | 0.56 | 1.295| 4.339|
| Ethylbenzoate (EBT)| 2.86        | −2.38          | 0.69           | 0.85 | 0.00 | 0.46 | 1.214| 5.075 |
| 4-nitrotoluol (4NT)| 2.65        | −2.76          | 0.87           | 1.11 | 0.00 | 0.28 | 1.032| 5.154 |
| 1-naphthol (1NP)  | 2.94        | 0.85           | 1.05           | 0.60 | 0.37 | 1.144| 6.284|
| 2-chlorophenol (2CP)| 4.05        | −3.24          | 0.85           | 0.88 | 0.32 | 0.31 | 0.898| 4.178 |

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* a solute descriptors were obtained from Ref. [2].
* b $S_w$: aqueous solubility [mg L$^{-1}$] at 25 °C from Ref. [3].
* c $K_{aw}$: air-water partitioning constant [–] from Ref. [4] or calculated using a combination of Eq. (6)–(15) and (6)–(17) from ref [4]: $K_{aw} = \frac{P_{(T)} \cdot L}{C_{sat} \cdot T \cdot R} \cdot \frac{1}{C_{138}}$
* d $K_{ow}$: octanol-water partitioning constant [–] from Ref. [3].
linear free-energy relationships for sorption of organic compounds by PS micro- and nanoplastics are given in Table 8. Fig. 2 visualizes the correlation between experimental distribution coefficients of probe sorbates by aged polystyrene microplastics and octanol-water partitioning coefficients.

### Table 2
Data of the Freundlich Model fit to the experimental sorption isotherms.

| Compound | $K_F$ | $n$ | $R^2$ | $N$ |
|----------|-------|-----|-------|-----|
| nHex     | 1.19E+04 ± 7.87E02 | 0.89 ± 0.02 | 0.956 | 15  |
| iHex     | 3.77E+03 ± 3.98E+02 | 1.11 ± 0.05 | 0.969 | 15  |
| cHex     | 4.19E+02 ± 8.44E+01 | 1.17 ± 0.04 | 0.989 | 13  |
| DCM      | 5.87E+01 ± 6.67E+00 | 0.92 ± 0.02 | 0.981 | 14  |
| TCM      | 1.69E+02 ± 2.58E+01 | 1.10 ± 0.03 | 0.985 | 15  |
| DPE      | 6.78E+01 ± 1.23E+01 | 1.01 ± 0.03 | 0.936 | 15  |
| 2ON      | 5.84E+01 ± 2.03E+01 | 1.07 ± 0.06 | 0.999 | 15  |
| HXN      | 5.54E+01 ± 2.30E+01 | 0.90 ± 0.06 | 0.935 | 15  |
| 1NH      | 3.07E+02 ± 1.50E+02 | 0.92 ± 0.07 | 0.968 | 10  |
| 2OL      | 2.13E+02 ± 5.47E+01 | 0.92 ± 0.06 | 0.917 | 10  |
| 3EH      | 5.81E+01 ± 1.61E+01 | 0.80 ± 0.05 | 0.967 | 14  |
| DMH      | 9.08E+01 ± 1.68E+01 | 0.81 ± 0.04 | 0.924 | 14  |
| BEZ      | 2.54E+02 ± 5.25E+01 | 0.94 ± 0.03 | 0.977 | 15  |
| TOL      | 3.37E+02 ± 7.68E+01 | 0.96 ± 0.03 | 0.920 | 15  |
| CBZ      | 1.80E+03 ± 1.83E+02 | 0.83 ± 0.02 | 0.961 | 15  |
| NAP      | 1.81E+03 ± 4.41E+02 | 1.02 ± 0.04 | 0.987 | 12  |
| BTZ      | 2.65E+02 ± 6.42E+01 | 1.00 ± 0.04 | 0.968 | 12  |
| EBT      | 1.20E+04 ± 3.50E+03 | 0.70 ± 0.04 | 0.954 | 11  |
| 4NT      | 3.15E+02 ± 1.70E+02 | 1.00 ± 0.07 | 0.980 | 11  |
| 1NT      | 6.72E+02 ± 2.21E+02 | 0.93 ± 0.05 | 0.952 | 9   |
| 2CP      | 3.78E+01 ± 1.37E+01 | 1.10 ± 0.05 | 0.946 | 14  |

$K_F$: Freundlich coefficient; $n$: Freundlich exponent; $R^2$: regression coefficient; $N$: number of data points.

2. Statistical analyses of ppLFER

See Table 4–8 and Fig. 2.
3. Experimental design, materials and methods

3.1. Materials

Polystyrene microplastics were purchased as a powder from Goodfellow Cambridge Ltd. (Huntingdon, UK.). The particles were sieved to a size fraction between 125 and 250 μm. The sorbates included apolar aliphatics, monopolar aliphatics, bipolar aliphatics, non-polar aromatics, monopolar aromatics, and bipolar aromatics (Table 1).

### Table 3
Comparison of Freundlich parameters obtained for pristine and aged polystyrene microplastic particles.

| Sorbate | Pristine PS | Aged PS |
|---------|-------------|---------|
|         | $K_F$ | $n$ | $R^2$ | $K_F$ | $n$ | $R^2$ |
| nHex    | 14,643.2 | 0.762 | 0.941 | 11,906.5 | 0.891* | 0.911 |
| cHex    | 2566.6   | 0.742 | 0.964 | 734.7 | 0.999* | 0.909 |
| BEZ     | 800.3    | 0.844 | 0.981 | 265.5** | 0.931** | 0.920 |
| CBZ     | 3421.1   | 0.810 | 0.971 | 1695.0** | 0.902** | 0.961 |
| NAP     | 2333.3   | 0.906 | 0.936 | 1806.2 | 0.999 | 0.917 |

* $p < 0.05$.
** $p < 0.01$.

### Table 4
Parameters for ppLFER using ESABV descriptors.

| Coefficient | SE | $p$-Value |
|-------------|----|-----------|
| $e$         | 0.6708 | 0.1613 | 0.0008 |
| $s$         | $-0.7491$ | 0.2012 | 0.0020 |
| $a$         | $-1.5278$ | 0.4399 | 0.0034 |
| $b$         | $-3.5158$ | 0.4110 | $<0.0001$ |
| $v$         | $2.8607$ | 0.3012 | $<0.0001$ |
| $c$         | $0.7365$ | 0.2510 | 0.0102 |

### Table 5
ANOVA for ppLFER using ESABV descriptors.

| df | SS  | MS  | $F$-value | $F$-critical |
|----|-----|-----|-----------|--------------|
| Model | 5   | 7.971 | 1.594 | 45.162 | 1.62E–08 |
| Residue | 15  | 0.5295 | 0.0353 | | |
| Total  | 20  | 8.500 | | | |

### Table 6
Parameters for ppLFER using SABVL descriptors.

| Coefficient | SE | $p$-Value |
|-------------|----|-----------|
| $s$         | $-0.10188$ | 0.3155 | 0.0056 |
| $a$         | $-1.4273$ | 0.4863 | 0.0102 |
| $b$         | $-3.6072$ | 0.4556 | $<0.0001$ |
| $v$         | $1.4481$ | 0.5748 | 0.0236 |
| $l$         | $0.4252$ | 0.1279 | 0.0046 |
| $c$         | $1.0089$ | 0.2979 | 0.0041 |
3.2. Aging of polystyrene microplastic particles

A custom-made aging chamber was used for particle aging. The particles were weighed into quartz glass petri dishes containing 50 mL of H₂O₂ (10 vol%). The samples were then irradiated for 96 hours using UV light (4*15 W UVC-bulbs, max. wavelength at 254 nm). The aged particles were washed with deionized water and dried prior to the sorption batch experiments.

### Table 8

| Sorbent                      | Sorbates             | opLFER                  | AIC       | RMSE     | N  |
|------------------------------|----------------------|-------------------------|-----------|----------|----|
| Aged PS microplastics [1]    | Non-ionic organics   | Log $K_d = 0.35 \pm 0.09$ log $K_{ow}$ + $1.63 \pm 0.24$ | $-52.63$  | $0.586$  | $21$ |
| Pristine PS microplastics [5]| Non-polar organics   | Log $K_d = 0.92$ log $K_{ow}$ + $0.31$ | $-24.85$  | $0.219$  | $7$  |
| Surface coated PS nanoplastics [6]| PCBs       | Log $K_d = 1.01$ log $K_{ow}$ + $0.36$ | $-69.46$  | $0.566$  | $17$ |
| Surface coated PS nanoplastics [7]| PAH      | Log $K_d = 0.65$ log $K_{ow}$ + $3.87$ | $-38.39$  | $0.131$  | $6$  |

AIC: Akaike’s Information Criterion; RMSE: root mean squared error; N: number of data points.

### Table 7

ANOVA for ppLFER using SABVL descriptors.

| df | SS   | MS  | $F$-value | $F$-critical |
|----|------|-----|-----------|--------------|
| Model | 5    | 7.844 | 1.569 | 35.841 | 7.97E−08 |
| Residue | 15   | 0.6565 | 0.0437 |           |           |
| Total | 20   | 8.5000 |       |           |           |

All parameters were calculated at a 95% confidence level.

SE: standard error of estimates.
df: degrees of freedom.
SS: sum of squares.
MS: mean square.

Fig. 2. Comparison between experimentally determined log $K_d$ and calculated by opLFER using log $K_{ow}$. AIC: Akaike’s Information Criterion; RMSE: root mean squared error; N: number of data points.

3.2. Aging of polystyrene microplastic particles

A custom-made aging chamber was used for particle aging. The particles were weighed into quartz glass petri dishes containing 50 mL of H₂O₂ (10 vol%). The samples were then irradiated for 96 hours using UV light (4*15 W UVC-bulbs, max. wavelength at 254 nm). The aged particles were washed with deionized water and dried prior to the sorption batch experiments.
3.3. Sorption experiments

20–60 mg of the sorbent particles were weighed into 20-mL amber headspace screw vials. 10 mL of 0.01 M CaCl₂ was added as background solution. The vials were closed with screw caps with butyl/PTFE-lined septa and wrapped in aluminum foil. After shaking overnight at 125 rpm to pre-wet the sorbent, the samples were spiked with sorbate standard solutions (methanol did not exceed 0.5%, to avoid co-solvent effects). The vials were then shaken for 7 days at 125 rpm for equilibration at a temperature of 25 ± 2 °C. Equilibration was determined using naphthalene as a probe sorbate (Fig. 1). The vials were then placed on the tray of the autosampler at least 2 hours prior to analysis. The concentrations in the head space of the vials was measured with a GC–MS-system either using in-tube microextraction or direct injection of 500 µL of the headspace sample. The sorbed concentrations were calculated using a mass balance and the air-water partitioning constants of the sorbates (Table 1).

3.4. Data analysis

Distribution coefficients between the aqueous phase and the sorbent (Kd) [L/kg] were calculated for all sorbates at a constant sorbate loading on aged PSMP of 1000 µg/kg, using the Freundlich equation:

\[
K_d = \frac{C_s}{C_w} = K_F C_w^{n-1}
\]

where \(C_s\) [µg/kg] and \(C_w\) [µg/L] are the sorbed and aqueous concentrations of sorbates at equilibrium, respectively, and \(K_F\) [(µg/kg)/(µg/L)\(^n\)] and \(n\) [-] are the Freundlich coefficient and exponent, respectively. Model parameters were obtained using Sigma Plot 12.0 software for Windows.

Declarations of interest

None.

Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2018.03.053.

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