

1 **Supporting Information for**

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3 **Dynamic Accumulation and Co-occurrence of Phthalates and Squalene**
4 **in Settled Dust: Implications for Assessing Indoor Phthalate Homology**
5 **and Exposures**

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7 Zhongming Bu¹, Donghui Mo¹, Yu Sun¹, Li Zhang², Yuqing Zhu², Xingyu Duan², Luying Nian²,

8 Yuanjun Tang¹, Chao Ye¹, Jianping Cao^{2,3,4,*}

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10 ¹ *Department of Energy and Environment System Engineering, Zhejiang University of Science and*
11 *Technology, Hangzhou 310023, China*

12 ² *School of Environmental Science and Engineering, Sun Yat-sen University, Guangzhou 510006,*
13 *China*

14 ³ *Southern Marine Science and Engineering Guangdong Laboratory (Zhuhai), Zhuhai 519082, China*

15 ⁴ *Institute of Carbon Neutrality and Green Development, Sun Yat-sen University, Guangzhou 510006,*
16 *China*

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18 *Corresponding email: caojp3@mail.sysu.edu.cn

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21 **This supporting information (7 pages) includes 2 sections, 3 tables and 1 figure.**

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23 Section S1. Detailed information of chemical analysis

24 All samples were analyzed using a GC-MS system (Agilent Technologies, GC-8890 & MS-5977B)
25 equipped with an auto-liquid injector (Agilent G4513A). For each sample vial, 1 μL extract was
26 injected into the GC injection port. A chromatographic column with the dimensions 30m \times 0.25mm
27 i.d. \times 0.25 μm film thickness (Agilent HP-5MS, Helium gas at 1.5 mL/min) was used for
28 chromatography separation. The temperatures of the injection port and ion source were 290 $^{\circ}\text{C}$ and
29 250 $^{\circ}\text{C}$, respectively. The GC oven temperature was maintained at 100 $^{\circ}\text{C}$ for 2 min, increased to 300
30 $^{\circ}\text{C}$ at 10 $^{\circ}\text{C}/\text{min}$ and then held for 5 min, i.e., totally 27 min. The MS worked with an electron collision
31 ionization (EI, 70 eV) and operated in both Scan (mass range 35-400 AMU) and SIM (Selected Ion
32 Monitoring) modes. The targeted compounds were quantified by the selected molecular ions: $m/z=105$
33 for benzyl benzoate (BB), $m/z=163$ for DMP, $m/z=129$ for DEHA, $m/z=149$ for other target phthalates,
34 $m/z=153$ for deuterated phthalates, and $m/z=69$ for squalene.

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36 A six-point calibration curve was prepared using standard mixture with concentrations of 1.0, 2.0, 4.0,
37 10, 20 and 40 $\mu\text{g}/\text{mL}$ (of each analyte). A total of 1 μg BB, 1 μg DnBP- d_4 and 1 μg DEHP- d_4 was
38 added to each 100 μL standard solutions. The ratio of each compound's peak area to the BB peak area
39 was linearly related to the ratio of each compound's amount to the BB amount. The linear function
40 was assumed valid when $R^2 > 0.99$. The limit of quantitation (LOQ) was 1 $\text{ng}/\mu\text{L}$ for 1 μL injection
41 (i.e., 1 ng).

42

43 According to Table S1, the concentrations of phthalates and squalene on the glass fiber filters can be
44 significantly reduced after high temperature baking and the treated fiber filters did not affect the
45 experimental results. In the formal experiment, we set up several blank samples: if the peak area ratio
46 of a certain compound measured in the dormitory dust was almost the same as the blank, the compound
47 was considered non-detected. It can be seen from the results that the detection rates of 8 compounds
48 in the blank experiment were close to zero.

49 **Table S1.** Amount (μg) of target compounds detected in blank samples ^a

		DMP	DEP	DiBP	DnBP	BBzP	DEHA	DEHP	DnOP	Squalene
Pilot trails ^b	HX	/	/	/	/	/	/	0.16	0.10	/
	HD	/	/	/	/	/	/	0.17	0.10	/
Field test	HD	/	/	<0.29	<0.47	/	<0.61	<0.98	<0.63	/

50 ^a “/” refers to “non-detected”; HX: extracts of the pretreated GF/A filter (47 mm diameter); HD:
 51 extracts of the pretreated GF/H filter (110 mm diameter).

52 ^b Values represent the means from 15 pilot trails.

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54 Section S2. Health burdens estimated from dust-phase levels

55 According to the Chinese Burden of Disease Attributable to Indoor Air Pollutants (CBD-IAP)¹
 56 research findings, as an example, asthma was chosen as the target health outcome associated with
 57 indoor phthalate exposure.² The burden of disease (BD) quantified by disability-adjusted life years
 58 (DALYs) was estimated as follows:

$$DALY = PAF \times DALY_{total} \quad (S1)$$

59 where *PAF* is the population attributable fraction corresponding to exposure associated with a given
 60 compound; and *DALY_{total}* is the total DALY value caused by asthma for the target population.

61

62 The *PAF* can be calculated as follows,

$$PAF = \frac{RR - 1}{RR} \quad (S2)$$

63 where *RR* is the relative risk for asthma, which is derived from the Concentration-Response curve (as
 64 a function of exposure level of dust-phase phthalate) reported by Liu et al.’s study, i.e.,²

$$RR = \begin{cases} RR_0 \frac{C}{\Delta C}, & C \leq C_{max} \\ RR_0 \frac{C_{max}}{\Delta C}, & C > C_{max} \end{cases} \quad (S3)$$

65 where *C* ($\mu\text{g}/\text{g}$) is the personal exposure concentration of dust-phase phthalate; *RR₀* is the relative risk
 66 for asthma, i.e., 1.04 (95%CI: 0.998,1.08) for DnBP and 1.001 (95%CI: 1.000-1.002) for DEHP,

67 respectively; ΔC is the unit gradient of concentration increase (10 $\mu\text{g/g}$ for DnBP, and 1 $\mu\text{g/g}$ for
 68 DEHP); and C_{max} ($\mu\text{g/g}$) is the upper bound of exposure level (291.9 $\mu\text{g/g}$ for DnBP, and 1648.6 $\mu\text{g/g}$
 69 for DEHP). Therefore, the disease burdens estimated by Eq. (S1) were closely linked with indoor dust-
 70 phase phthalate concentrations. For a specific population and health outcome, the disease burden is
 71 proportional to the *PAF*. In this study, we used median concentrations in settled dust as proxies for
 72 human exposure levels. Focusing on DnBP and DEHP as representative compounds, we calculated
 73 their corresponding *PAF* values, which are summarized in Table S2.

74

75 **Table S2.** Key parameters for health burden estimates based on dust-phase phthalate levels

		Dust-phase level ($\mu\text{g/g}$)	<i>RR</i>	<i>PAF</i>	Relative difference
DnBP	Sampling #1	57	1.251	0.200	-11.0%
	Sampling #2	65	1.290	0.225	/
	Sampling #3	73	1.332	0.249	10.6%
DEHP	Sampling #1	235	1.265	0.209	-27.9%
	Sampling #2	343	1.409	0.290	/
	Sampling #3	332	1.394	0.282	-2.7%

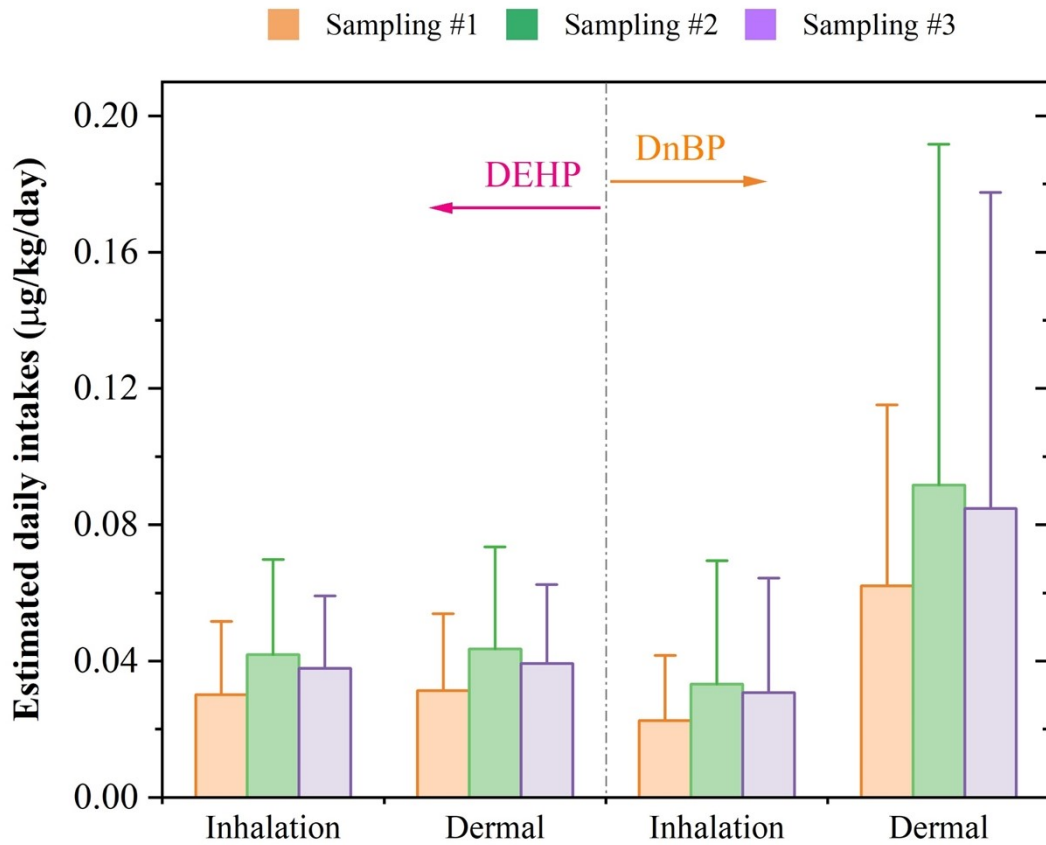
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77 **Table S3.** Exposure factors used for exposure estimates.

	Equations or parameters
Inhalation ^a	$DI_{inh} = \frac{(C_g + C_{sp}) \times IR_{inh} \times EF}{BW}$
Dermal absorption ^a	$DI_{derm-gas} = \frac{C_g \times k_{p-g} \times SA \times EF}{BW}$
Inhalation rate (IR_{inh} , m ³ /day) ^b	18.9
Body weight (BW , kg) ^b	68.6
Transdermal coefficient (k_{p-g} , m/day) ^c	DnBP: 115.2 DEHP: 139.2
Skin surface area exposed to air (SA , m ²) ^b	0.51
Exposure frequency (EF , unitless) ^d	0.625

78 ^a Exposure models were detailed elsewhere.³ ^b Values for adults were from Bu et al.'s study.⁴ ^c Based
 79 on Weschler and Nazaroff.⁵ ^d Assuming students spend 15 hours per day inside their dormitories.

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82 **Figure S1.** Inhalation and dermal exposure estimated by different measurement datasets. Sampling
 83 #1–3 correspond to February, March and April sampling. Exposure model and key parameters are
 84 detailed in Table S3.

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