## The Human Exposure Characteristics of Liquid crystal monomers (LCMs) and their mechanisms to cross the skin barrier

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*INTRODUCTION*: Liquid crystal monomers (LCMs) are persistent, bio-accumulative, and toxic substances widely used in liquid crystal displays of smart devices. However, little has been known about the human exposure and health risks of LCMs. Herein, the human exposure characteristics of LCMs and their mechanisms to cross the skin barrier were explored.

*METHODS*: A suite of 60 LCMs were selected as target compounds. 149 dust samples and 43 paired hand-forehead wipe samples of the workers were collected from October to November 2020 in an e-waste recycling industrial park in Central China. 48 indoor and 97 outdoor dust samples were collected across mainland China from March to August 2017. Estimated daily intake (EDI) based on the above samples was evaluated to assess the workers' and residents' exposure risks of LCMs. 3D-Human Skin Equivalents were used to assess the percutaneous penetration of LCMs quantitatively. The transporters in the skin were explored by molecular docking analysis.

**RESULTS:** LCMs were widely detected not only in e-waste areas but also in residents indoors and outdoors. The median EDI of the total LCMs ( $\Sigma$ LCMs) via dust ingestion and dermal contact of workers were 48.3 and 16.5 ng/kg BW/day, respectively, indicating a high occupational exposure risk of LCMs (Figure 1). The median EDI of  $\Sigma$ LCMs via dust ingestion, dermal contact, and inhalation of residents were 1.50 × 10<sup>-2</sup>, 2.90 × 10<sup>-2</sup>, and 8.57 × 10<sup>-6</sup> ng/kg BW/day, suggesting exposure risks of LCMs to residents (Figure 2). LCMs with higher log  $K_{ow}$  and molecular weight were more difficult to cross the skin barrier (Figure 3). And ABCG2 (an efflux transporter) may be responsible for the percutaneous penetration of LCMs (Figure 4).

*CONCLUSIONS*: There were exposure risks to both workers and residents of LCMs. Passive diffusion and active transport may be involved in the percutaneous penetration of LCMs.

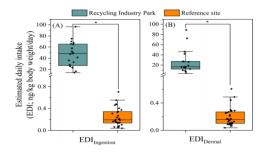


Figure 1. Estimated daily intake (EDI, ng/kg body weight/day) of occupational workers in a recycling industrial park and residents in a reference site of LCMs via (A) dust ingestion and (B) dermal exposure (asterisks (\*) represent significance levels with p < 0.05).

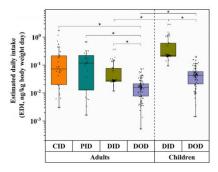


Figure 2. Estimated daily intake (ng/kg body weight/day) of LCMs for adults and children (asterisks (\*) represent significance levels with p < 0.05, DID, DOD, CID, and PID represent indoor dust, outdoor dust, indoor dust form cybercafe, and phone repair store, respectively).

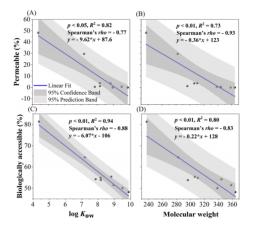


Figure 3. Correlation of permeable (% of total measured mass present in the receptor compartment) following the 36 h exposure with (A) log  $K_{ow}$  and (B) molecular weight, biologically accessible (% of total measured mass present in the receptor compartment and the skin tissue) following the 36 h exposure with (C) log  $K_{ow}$  and (D) molecular weight (of the applied 500 ng/cm<sup>2</sup> dose).

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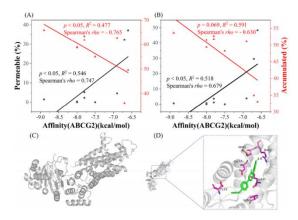


Figure 4. Correlation of permeable (% of total measured mass present in the receptor compartment) and accumulated (% of total measured mass accumulated in the skin tissue) following the 36 h exposure with the affinity of LCMs with ABCG2 of the applied (A) 500 ng/cm<sup>2</sup> and (B) 220 ng/ cm<sup>2</sup> doses; (C) protein structure of ABCG2; (D) docking results of ABCG2 and LCM.