Sorption behavior of hexabromocyclododecanes (HBCDs) on Weihe River sediment

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Analytical methods

The α-HBCD, β-HBCD, and γ-HBCD concentrations in each sample were determined using a high-performance liquid chromatography coupled to a triple quadrupole mass spectrometer (Agilent 6470 TSQ). The HBCDs stereoisomers were separated using a C18 column (2.1 mm i.d., 150 mm long, 3.0 μm particle size; Agilent, USA). During an analytical run, the column temperature was kept at 40 °C. The injection volume was 5.0 μL. Three mobile phases were used (A) acetonitrile, (B) methanol, and (C) water, and the flow rate was 0.3 mL/min. The mobile phase gradient program started at an A/B/C ratio of 55/20/25 (v/v/v), then changed in a linear fashion to an A/B/C ratio of 70/20/10 (v/v/v) over a period of 12.0 min, then changed to an A/B/C ratio of 100/0/00 (v/v/v) over 0.2 min. This A/B/C ratio was maintained for 8 min, then the A/B/C ratio changed to 55/20/25 (v/v/v), which was maintained for 9 min.

The mass spectrometer was operated in electrospray negative ionization mode, and the method used was based on previously published methods [24, 25]. The triple quadrupole mass spectrometer was operated in selected reaction monitoring mode. The capillary temperature and capillary spray voltage were 230 °C and 3.0 kV, respectively. The sheath gas and auxiliary gas were nitrogen, and the pressures were 28 psi and 5 psi, respectively. The tube lens offset was 80. The $[M-H]^- \rightarrow Br^-$ transitions m/z 640.2 → 81.0/642.2 → 81.0 were monitored.

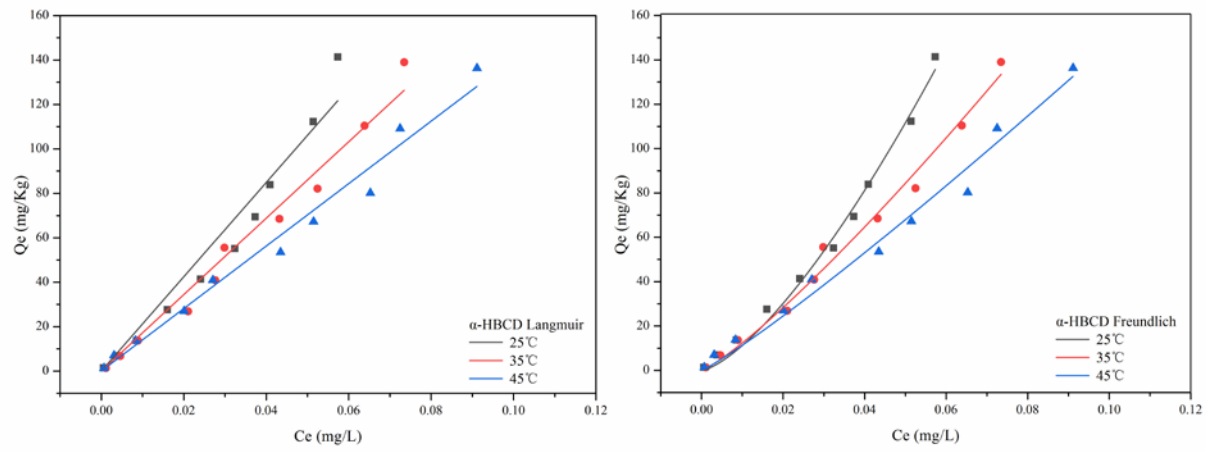

Figure S1. Sorption isotherms of α-HBCD in the sediment at different temperatures.

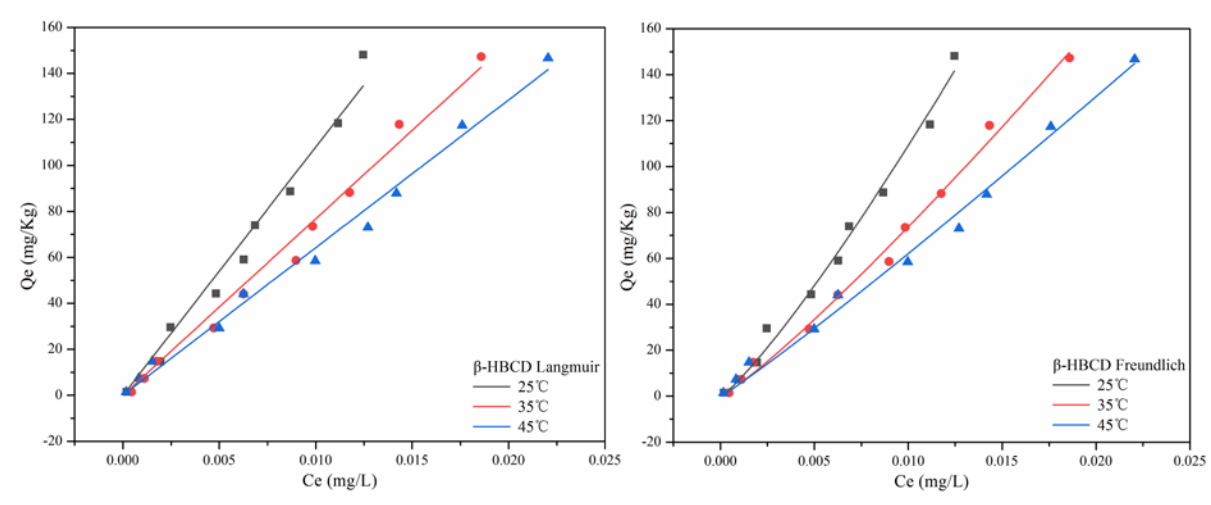

Figure S2. Sorption isotherms of β-HBCD in the sediment at different temperatures.

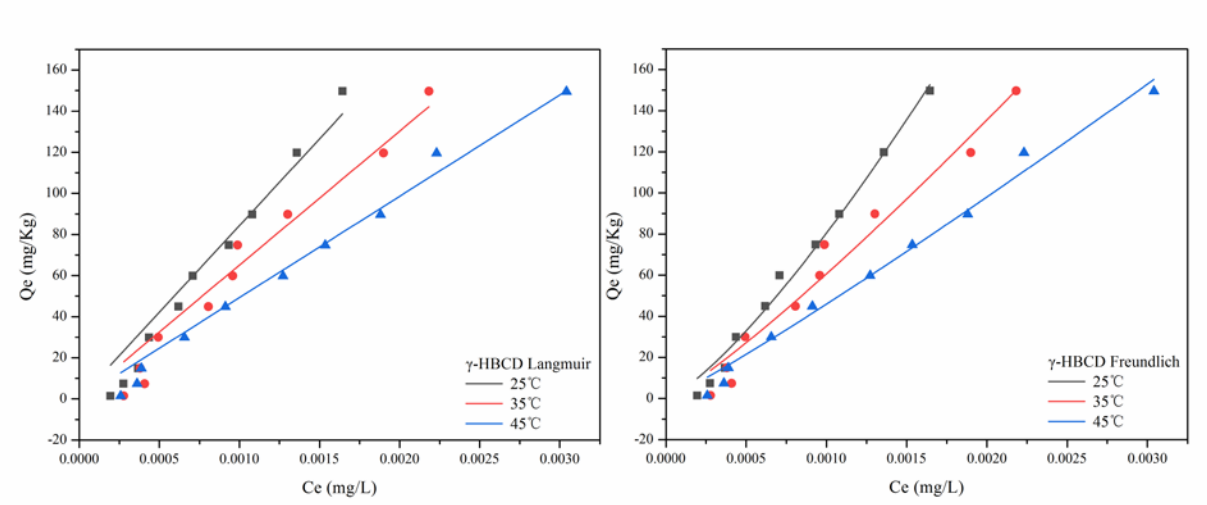

Figure S3. Sorption isotherms of γ-HBCD in the sediment at different temperatures.

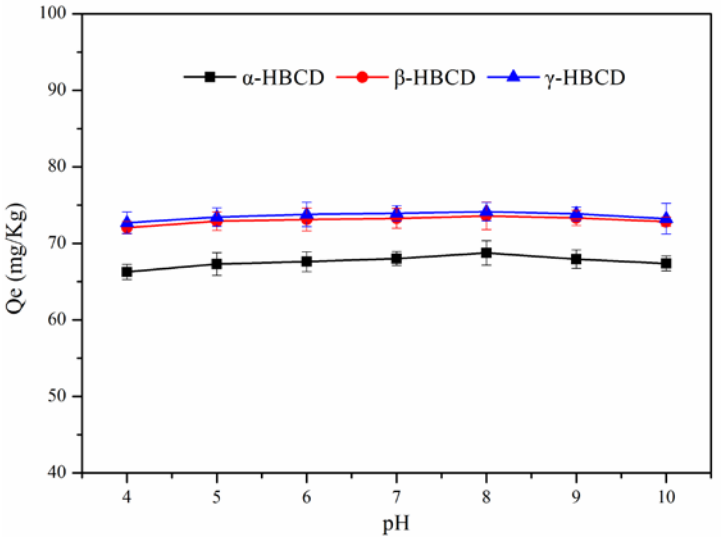

Figure S4. Effects of pH on HBCDs sorption in the sediment.

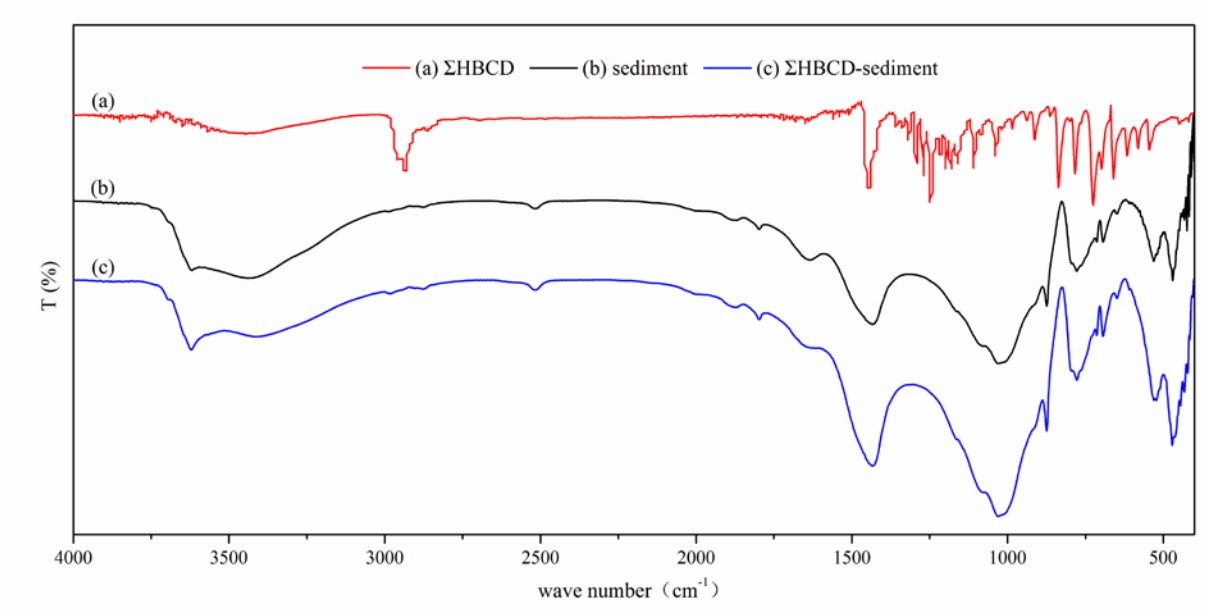

Figure S5. FTIR spectra of (a)∑HBCD, (b)sediment, (c)∑HBCD-sediment.