Supporting information

Engineering of efficient functionalization in a zirconium-hydroxyl-based metal-organic framework for ultra-high adsorption of Pb^{2+} ion from an aqueous medium: an elucidated uptake mechanism

Hang M. N. Pham,[a] Anh V. N. Phan,[a] Anh N. T. Phan,[a] Vi P. Nguyen,[a] Khang M. V. Nguyen,[a] Hung N. Nguyen,[a] Thai M. Nguyen[a] and My V. Nguyen*[a]

[a] Faculty of Chemistry, Ho Chi Minh City University of Education, Ho Chi Minh City, 700000, Vietnam.

*To whom correspondence should be addressed: mynv@hcmue.edu.vn

Keywords: OH-modified Zr-MOFs, Adsorption of Pb^{2+}, Heavy metal ion, Uptake mechanism, Treatment of wastewater.

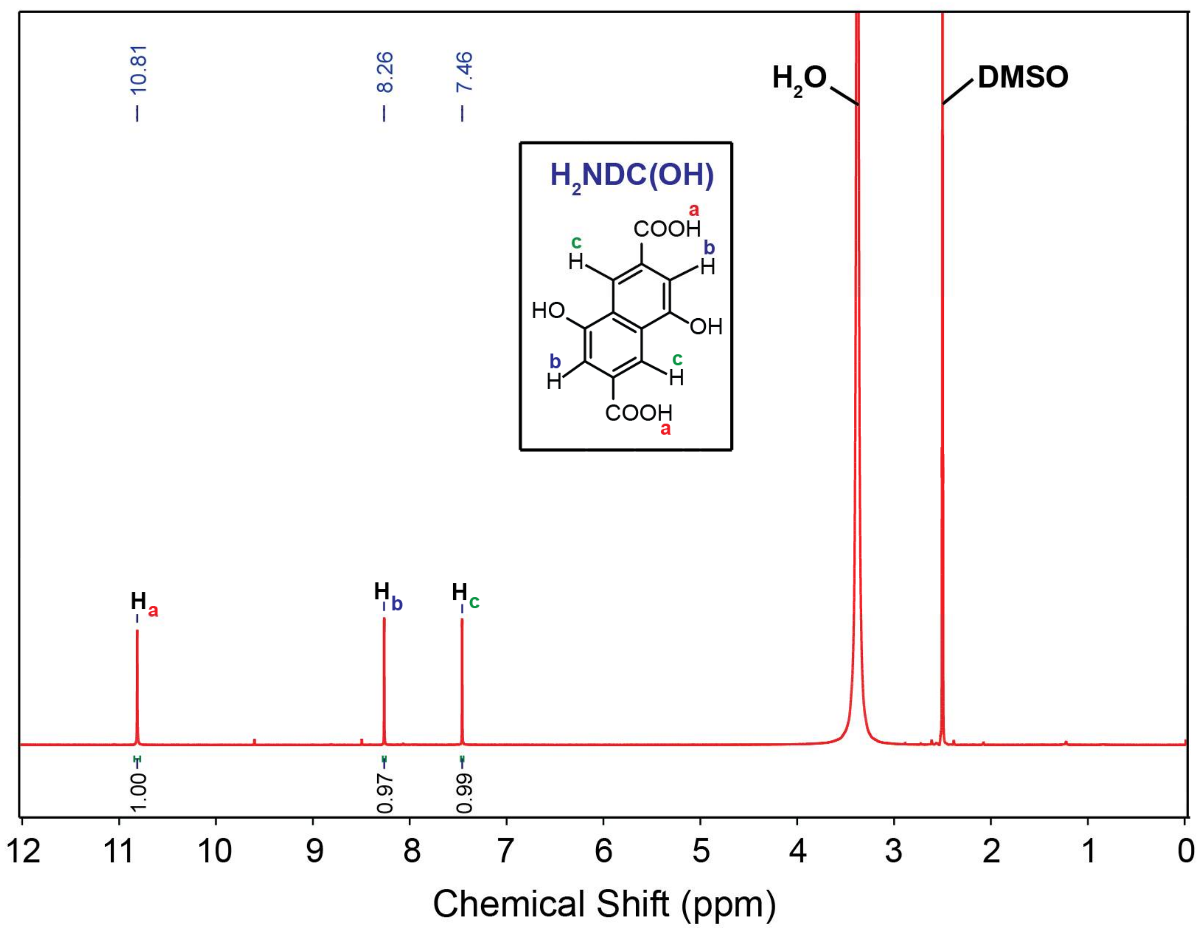

Figure S1. ^{1}H-NMR spectrum of $H_2NDC(OH)$ linker in DMSO solvent

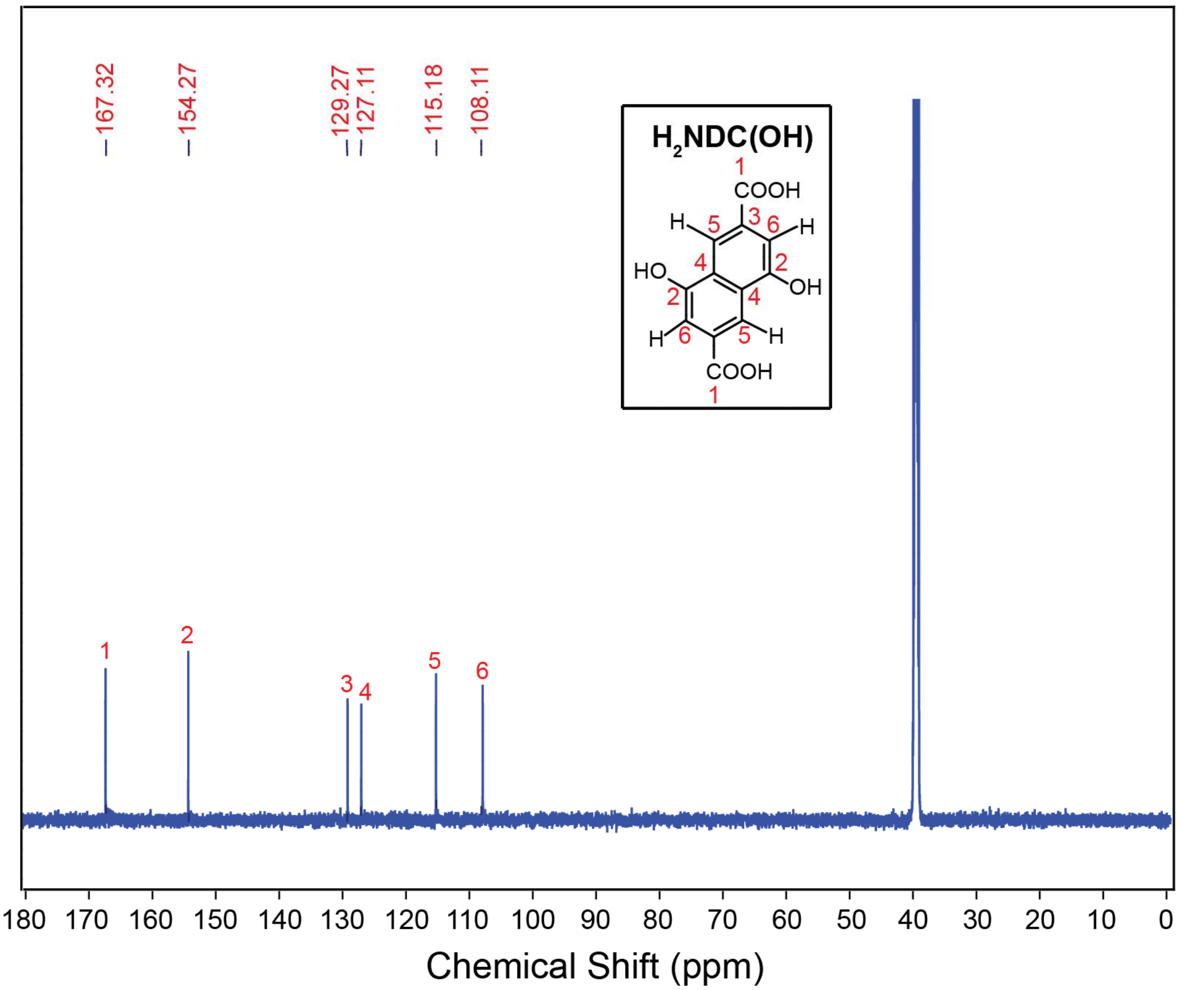

Figure S2. ^{13}C-NMR spectrum of $H_2NDC(OH)$ linker in DMSO solvent

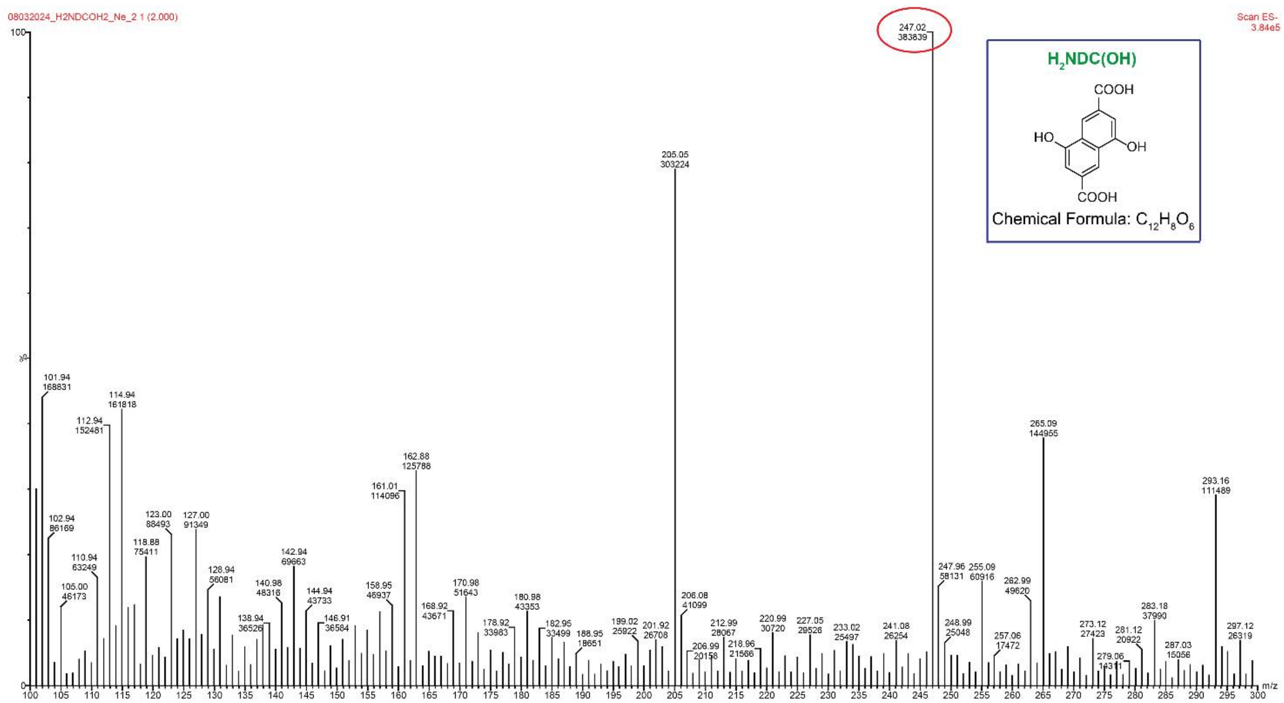

Figure S3. Mass spectroscopy of H_2NDC(OH) linker

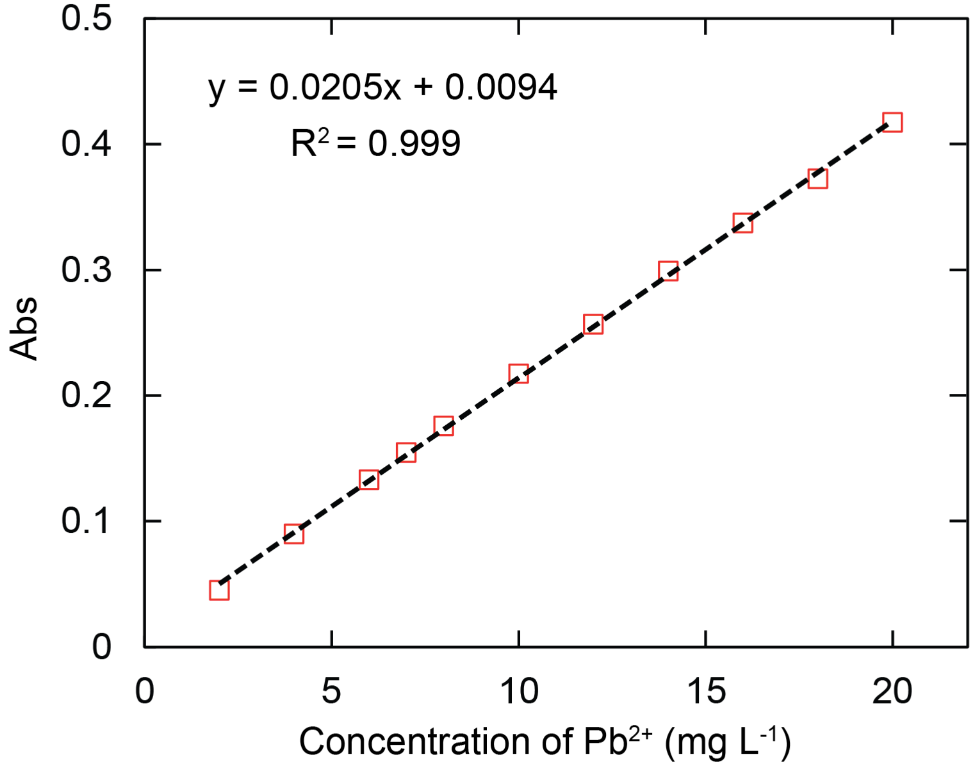

Figure S4. The relationship between the absorbed intensity of Pb^{2+} and various concentrations of 0 - 20 mg L^{-1} by linear fitting

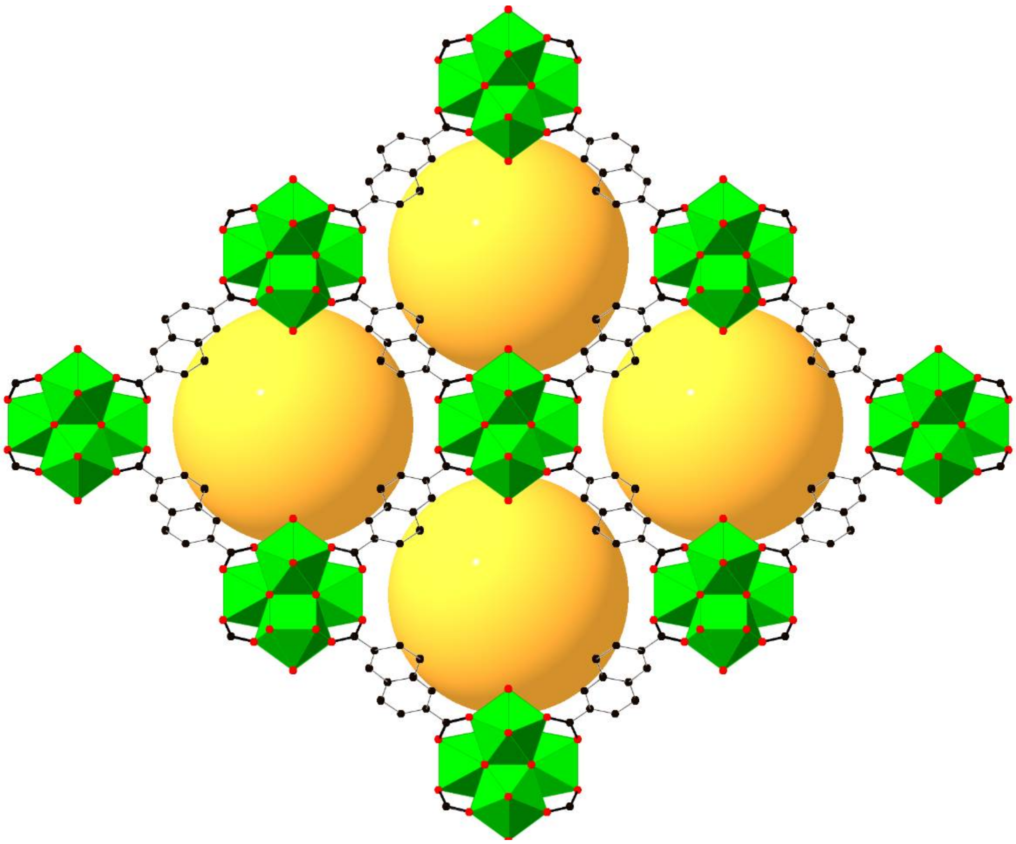

Figure S5. The structure of the Zr-bcu-NDC backbones is constructed from the $Zr_6O_8(H_2O)_8(CO_2)_8$ SBUs with the H_2NDC linker. Atom colors: Zr polyhedra, green; C, black; O, red. All H atoms are omitted for clarity.

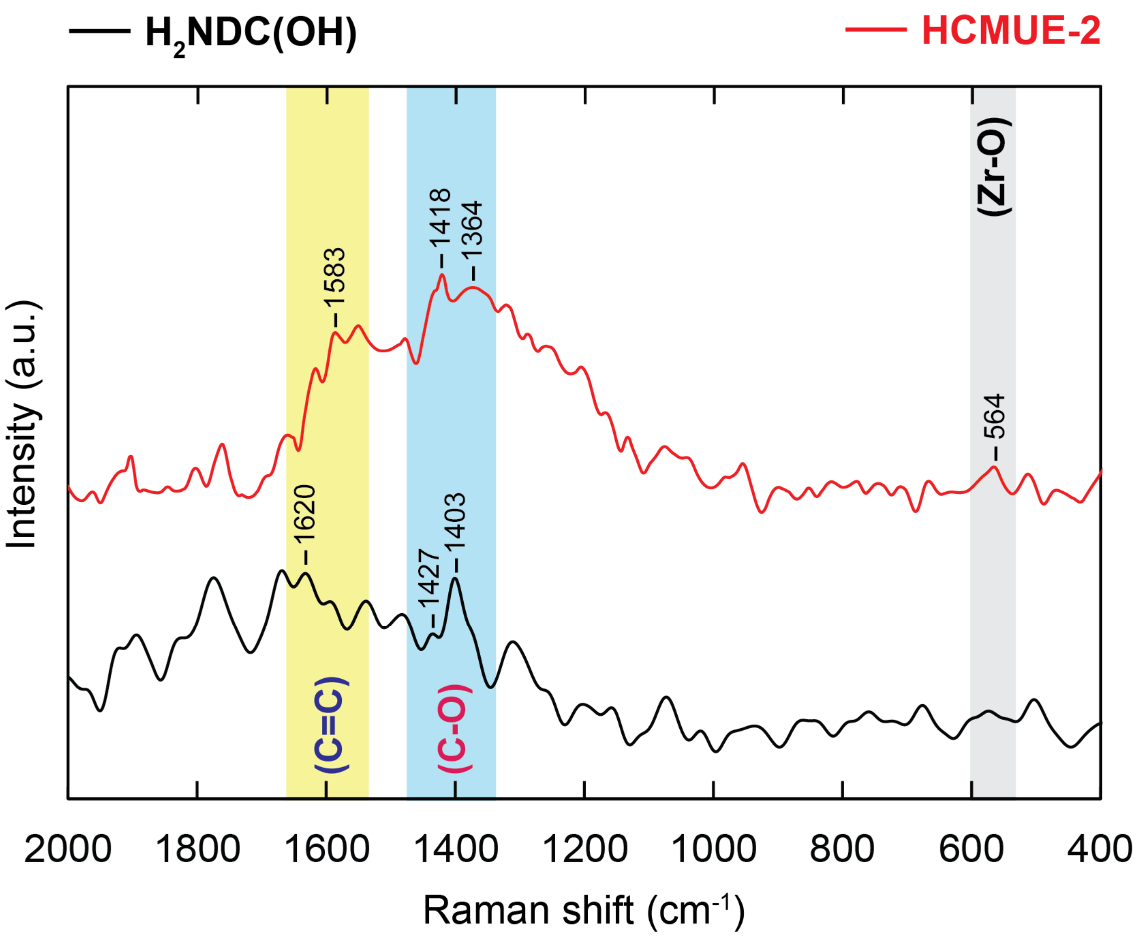

Figure S6. Raman spectrum of activated HCMUE-2 (red) in comparison with $H_2NDC(OH)$ linker (black)

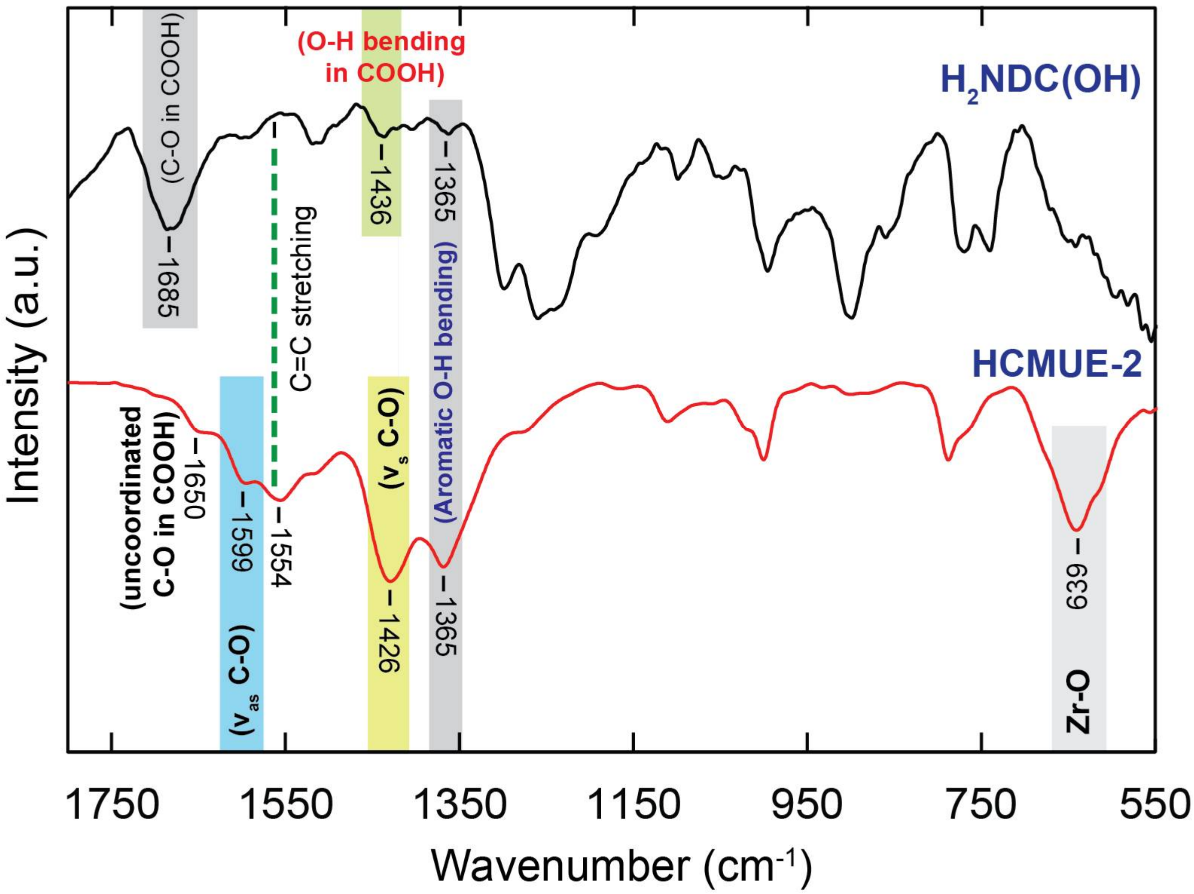

Figure S7. The FT-IR spectrum of HCMUE-2 (red) in comparison with $H_2NDC(OH)$ (black)

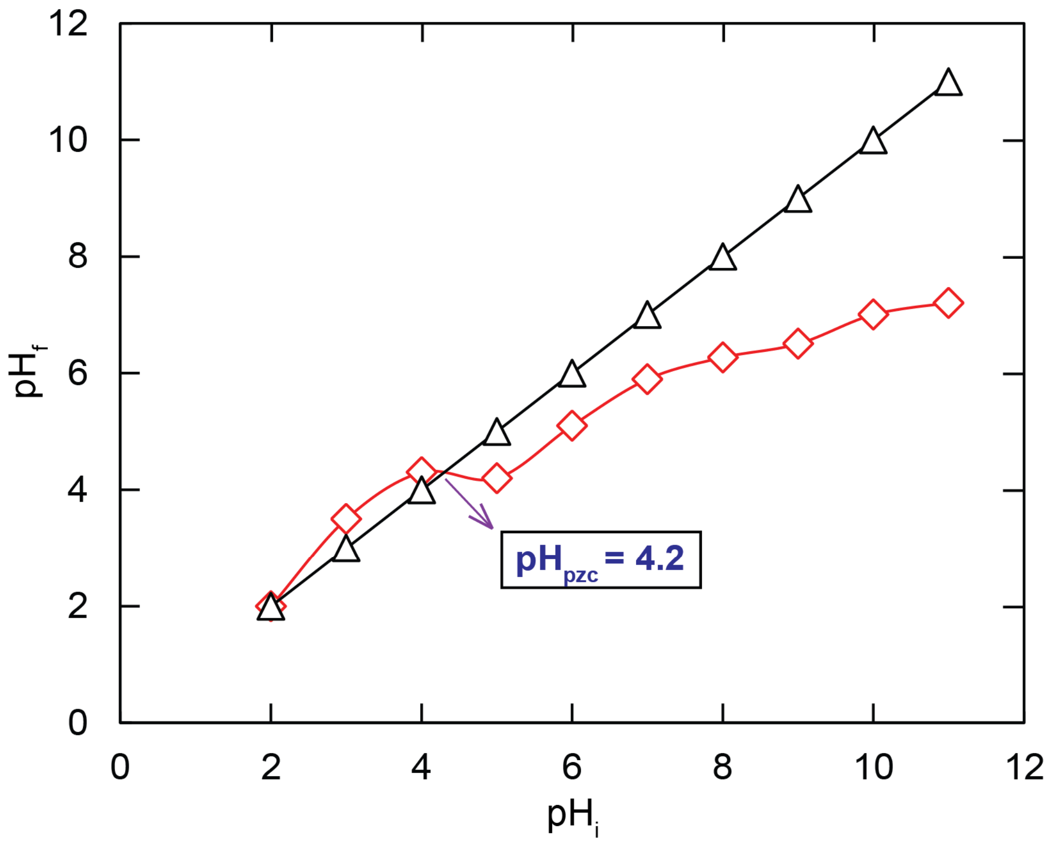

Figure S8. The effect of the initial pH on the final pH for determining pH_{pzc} of HCMUE-2. In detail, HCMUE-2 (150 mg) was introduced to 100 mL of glass bottles containing 50 mL of 0.01 M NaCl solutions with different initial pH ranges (pH_i) from 2 to 11. The mixtures were stirred for 48 h. The final pH value (pH_f) of the solutions was recorded using a pH meter. The intersection points between pH_i and pH_f values exhibited the pH_{pzc} value

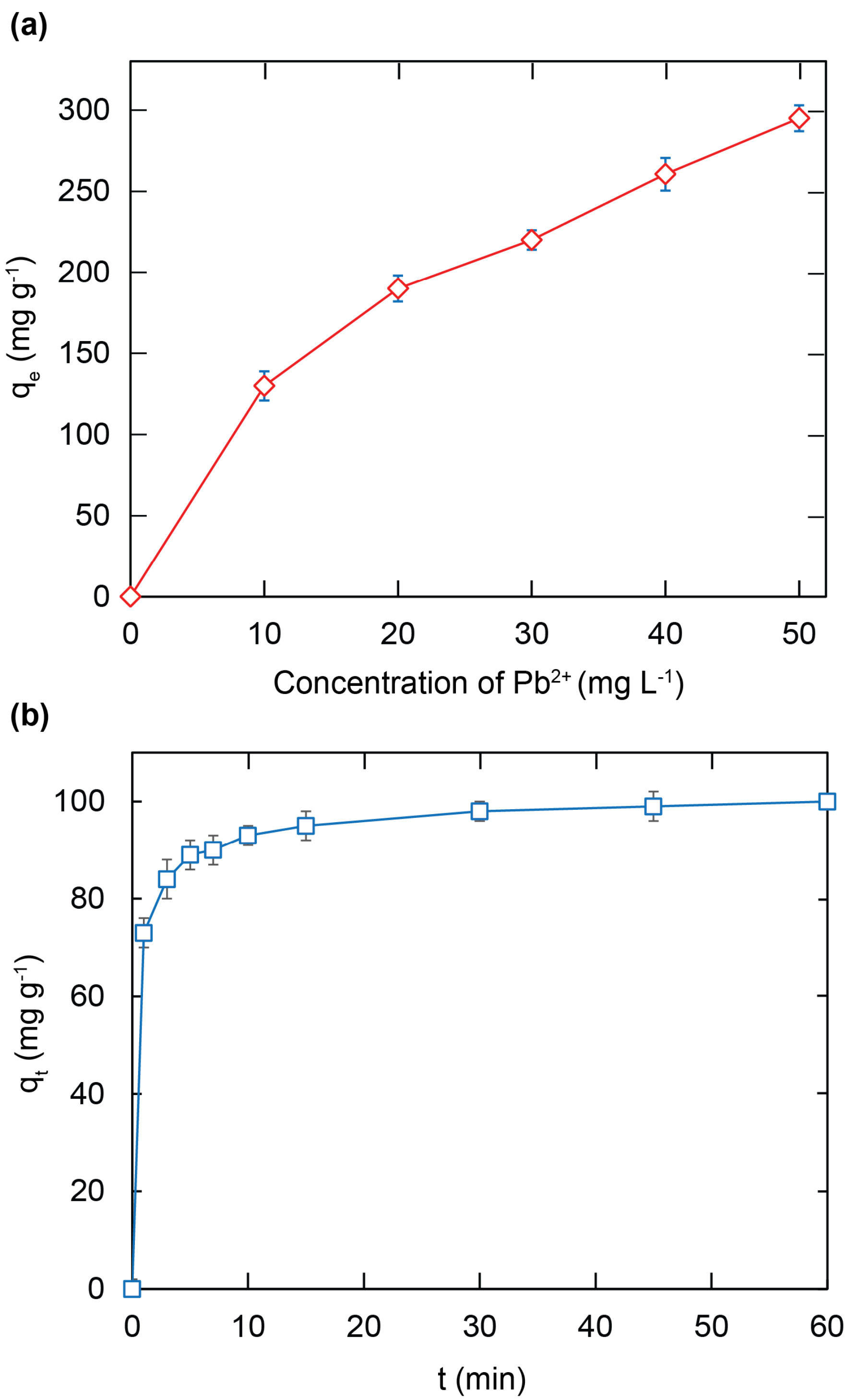

Figure S9. Effect of low initial concentrations on the adsorption uptake of Pb^{2+} over HCMUE-2 [m = 15 mg, V = 100 mL, C_o: 10 - 50 mg L^{-1}, pH = 5.5, t = 24 h] (a); The kinetic curve for the adsorption of Pb^{2+} at low concentrations onto HCMUE-2 [m = 5 mg, V = 50 mL, C_o = 10 mg L^{-1}, t = 1 - 60 min, pH = 5] (b)

Adsorption kinetics

The pseudo-first-order, pseudo-second-order, and intra-particle diffusion models are determined the equations (S1), (S2), and (S3):

$$q_t = q_e.(1 - e^{-k_1 t}) \qquad \text{(S1)}$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \qquad \text{(S2)}$$

$$q_t = k_i t^{1/2} + c \qquad \text{(S3)}$$

Where q_t (mg g^{-1}) and q_e (mg g^{-1}) symbolize the Pb^{2+} adsorption capacity at t and equilibrium time, respectively. k_1 (min^{-1}), k_2 (g mg^{-1} min^{-1}), and k_i (g mg^{-1} min^{-1}) represent the rate constants of pseudo-first-order, pseudo-second-order, and intra-particle diffusion models, and c is the constant, exhibiting the boundary layer thickness.