Supporting Information

Enhanced U(VI) Removal from Groundwater Using Amide-Functionalised Biopolymer-Based Adsorbent for a Practical Solution

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Supporting information content

Total number of pages: 19

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Equation (1): The fraction (%) of U(VI) adsorbed by CMABCH at different time intervals were calculated from IR spectra using the equation below

1a
$$x(t) = \frac{\Delta A(1)}{\Delta A(2)} \times 100$$

where x(t) is the fraction of U(VI) adsorbed at time t, ΔA(1) is the difference between adsorption at specific time t and one at time 0 and ΔA(2) is the corresponding value for the difference between adsorption at time 0 and completely adsorbed U(VI). Similarly, residual U(VI) fraction in water is calculated by firstly measuring the leftover concentration of U(VI) in water through ICP-MS and then the fraction of residual U(VI) was calculated using the equation below

1b
$$y(t) = (1 - \frac{\Delta A(1)}{\Delta A(2)}) \times 100$$

where y(t) is the residual fraction of U(VI) at time t, ΔA(1) is the difference between adsorption at specific time t and one at time 0 and ΔA(2) is the corresponding value for the difference between adsorption at time 0 and completely adsorbed U(VI).

Equation (2): The maximum uptake capacity (q_e) of U(VI) was determined by the equation below

$$\text{Uptake } (q_e) = \frac{(C_o - C_e)V}{m}$$

where q_e is the amount of U(VI) ions adsorbed per gram of adsorbent (mg/g) at equilibrium concentration, C_e is the equilibrium concentration of U(VI) in the bulk solution (mg/L), C_o is the initial U(VI) concentration (mg/L), V is the volume of solution (L) and m is the mass of adsorbent (g).

Equation (3): Ho's pseudo-second-order equation is described as

$$\frac{t}{q_e} = \frac{1}{k_2\, q_e^2} + \frac{1}{q_e} t$$

where q_e is the amount of U(VI) ions adsorbed per gram of adsorbent (mg/g), k_2 (g/mg/min) is the pseudo-second-order rate constant.

Equation (4): The linear form of Langmuir equation used

$$\frac{C_e}{q_e} = \frac{C_e}{q_{max}} + \frac{1}{bq_{max}}$$

where q_e is the amount of U(VI) ions adsorbed per gram of adsorbent (mg/g), C_e is the equilibrium concentration of U(VI) in the bulk solution (mg/L), q_{max} is the maximum surface density at monolayer coverage and b is the Langmuir adsorption constant (L/mg) related to the free energy of adsorption and $1/q_{max}$ and $1/bq_{max}$ are Langmuir constants.

Equation (5): Freundlich adsorption isotherm model was applied and the linear form of the equation used was

$$\log(q_e) = \log k_f + \frac{1}{n}\log\,(C_e)$$

where q_e is the amount of U(VI) ions adsorbed per gram of adsorbent (mg/g), C_e is the equilibrium concentration of U(VI) in the bulk solution (mg/L), k_f (mg/g) is the multilayer adsorption capacity and n is the empirical parameter connected with intensity of adsorption.

Equation (6): Mass intensity =

$$\frac{\text{mass of all products used excluding water}}{\text{mass of product}}\ \text{kg/kg product}$$

Equation (7): Water intensity (W_p) =

$$\frac{\text{mass of all water used}}{\text{mass of product}}\ \text{kg/kg product}$$

Equation (8): Reaction mass efficiency (RME) =

$$\frac{\text{mass of product}}{\text{mass of all reactants}} \times 100\%$$

Equation (9): E factor =

$$\frac{[\text{Kg(raw materials)} - \text{Kg(desired product)}]}{\text{Kg(total product including water)}}$$

Supporting Information 1

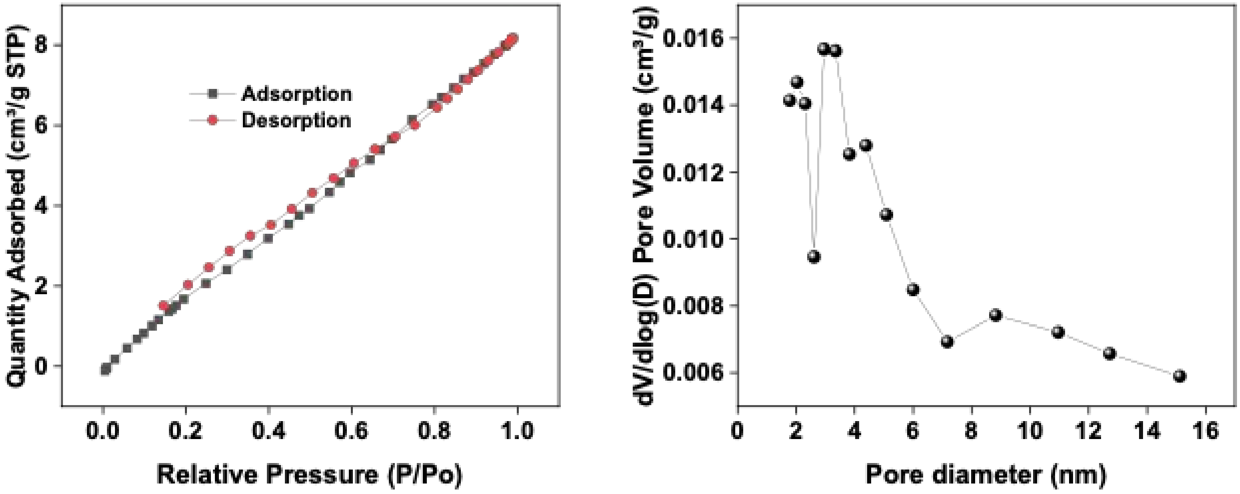

Figure S1. BET surface area (a) N_2 adsorption-desorption plot. (b) Pore size distribution.

Supporting Information 2

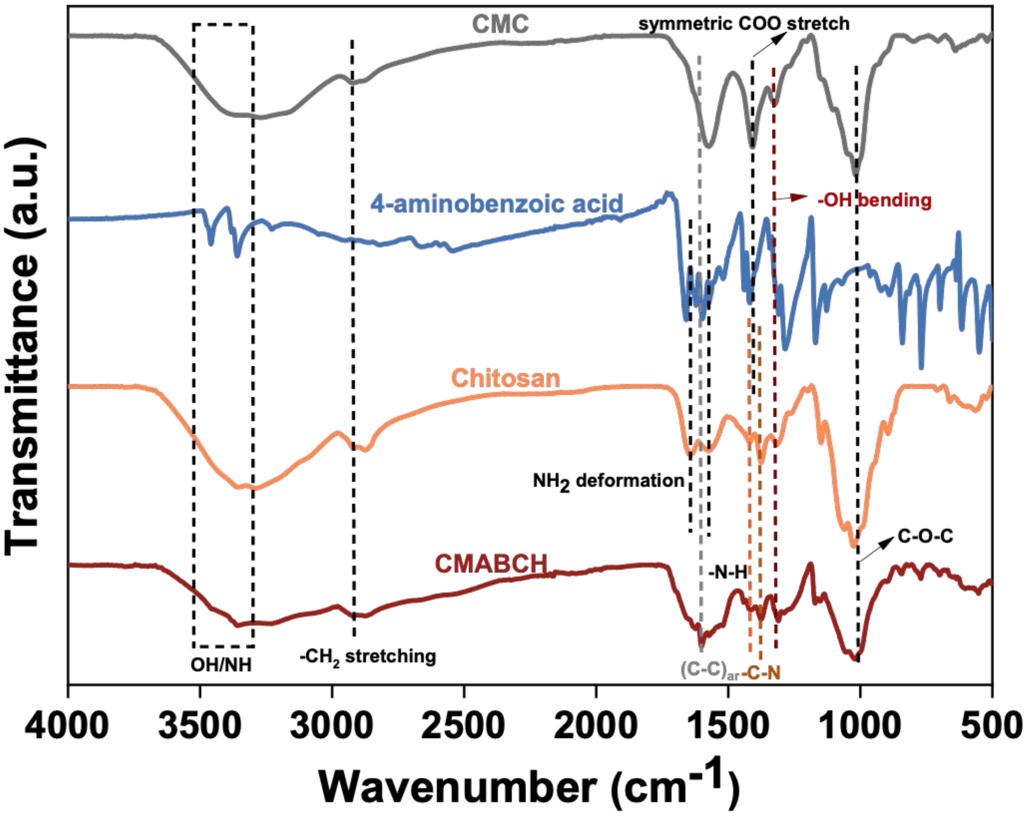

Figure S2. IR spectra of CMABCH and its precursors i.e., CMC, PABA, and CH.

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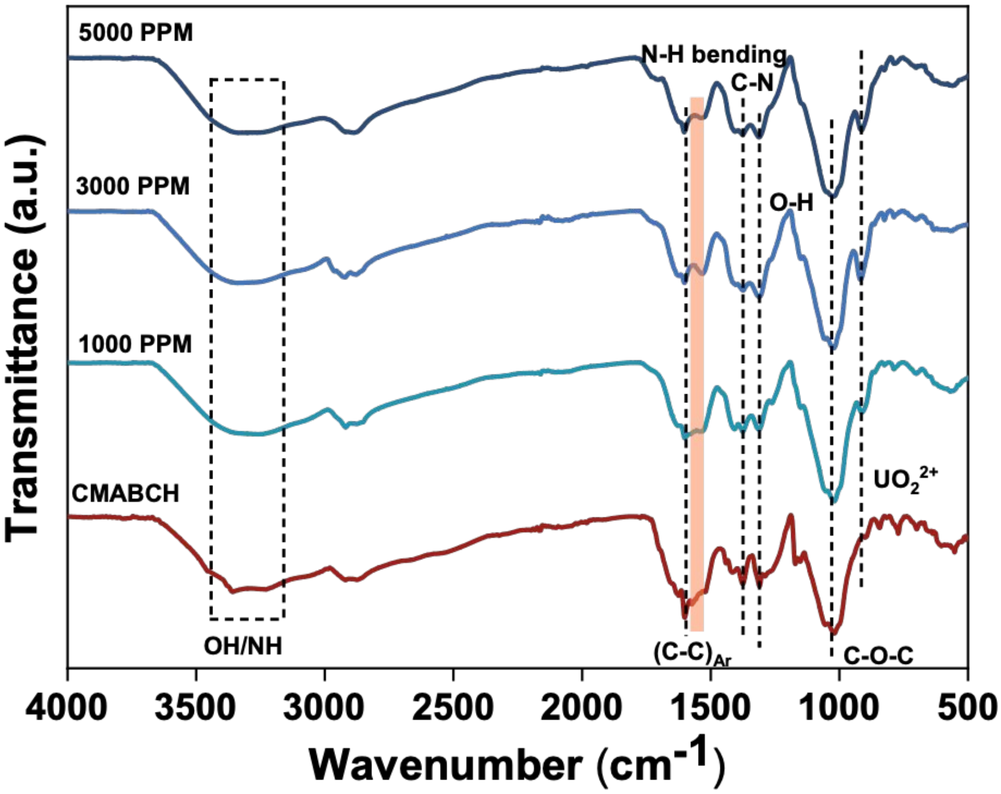

Figure S3. IR spectra of CMABCH, before and after treatment with various concentrations of U(VI) (m-50 mg, V-10 mL, pH-7).

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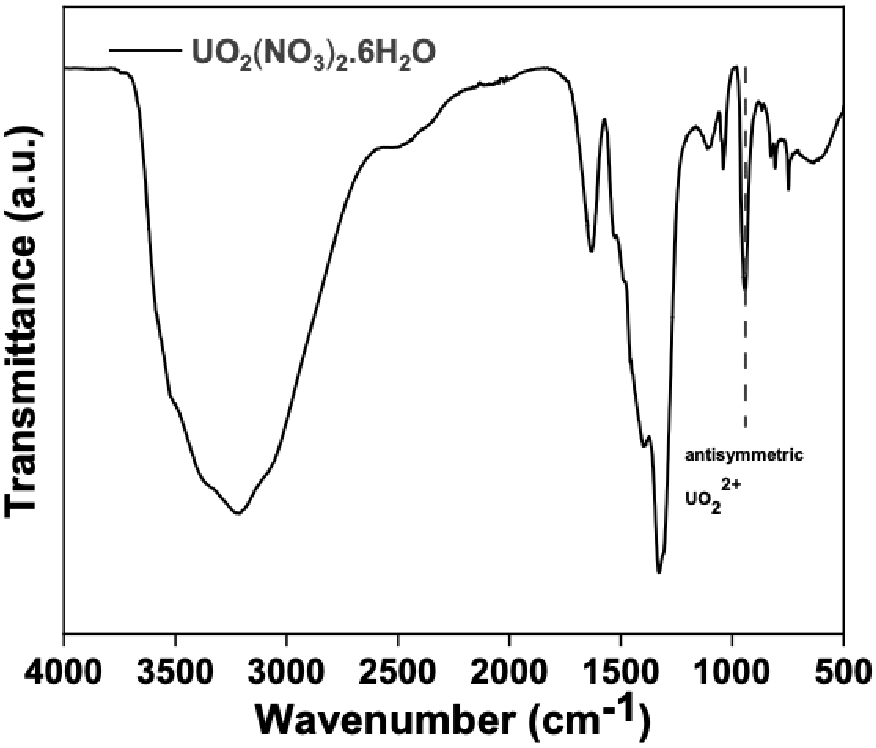

Figure S4. IR spectra of standard ($UO_2(NO_3)_2.6H_2O$).

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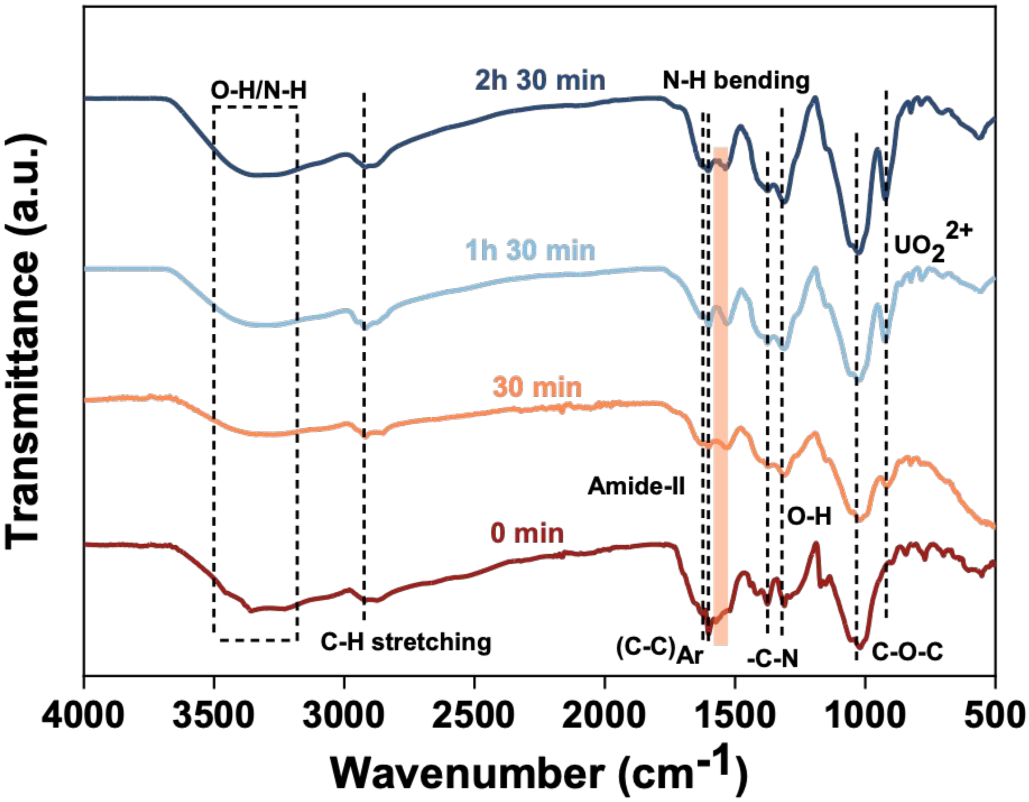

Figure S3. IR spectra of CMABCH, before and after U(VI) adsorption, at regular time intervals ($(U(VI))_o$- 5000 mg/L, m- 50 mg, V-10 mL, pH-7).

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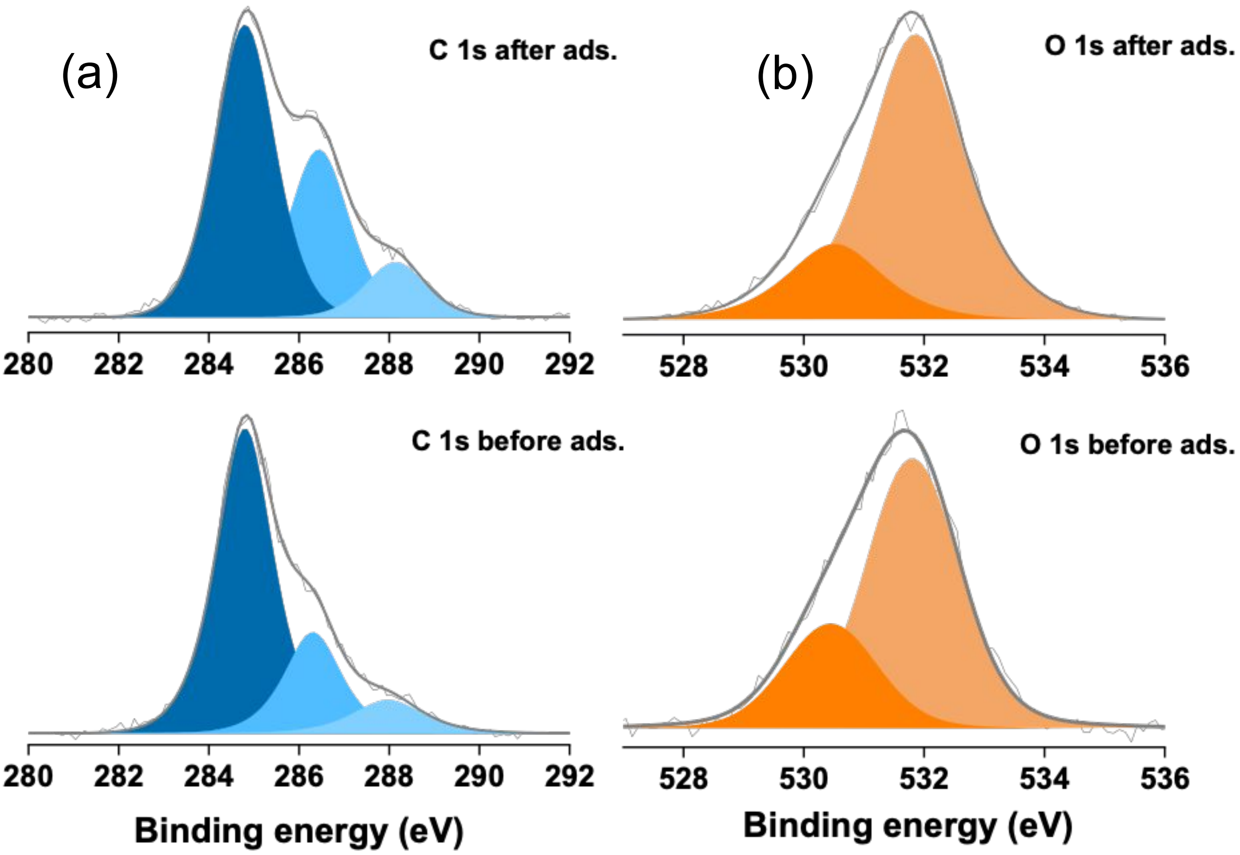

Figure S6. Deconvoluted XPS spectra of (a) C 1s and (b) O 1s regions of CMCBACH, before and after U(VI) adsorption (bottom to top). ($U(VI)_o$-5000 mg/L, m-50 mg, V-10 mL, pH-7).

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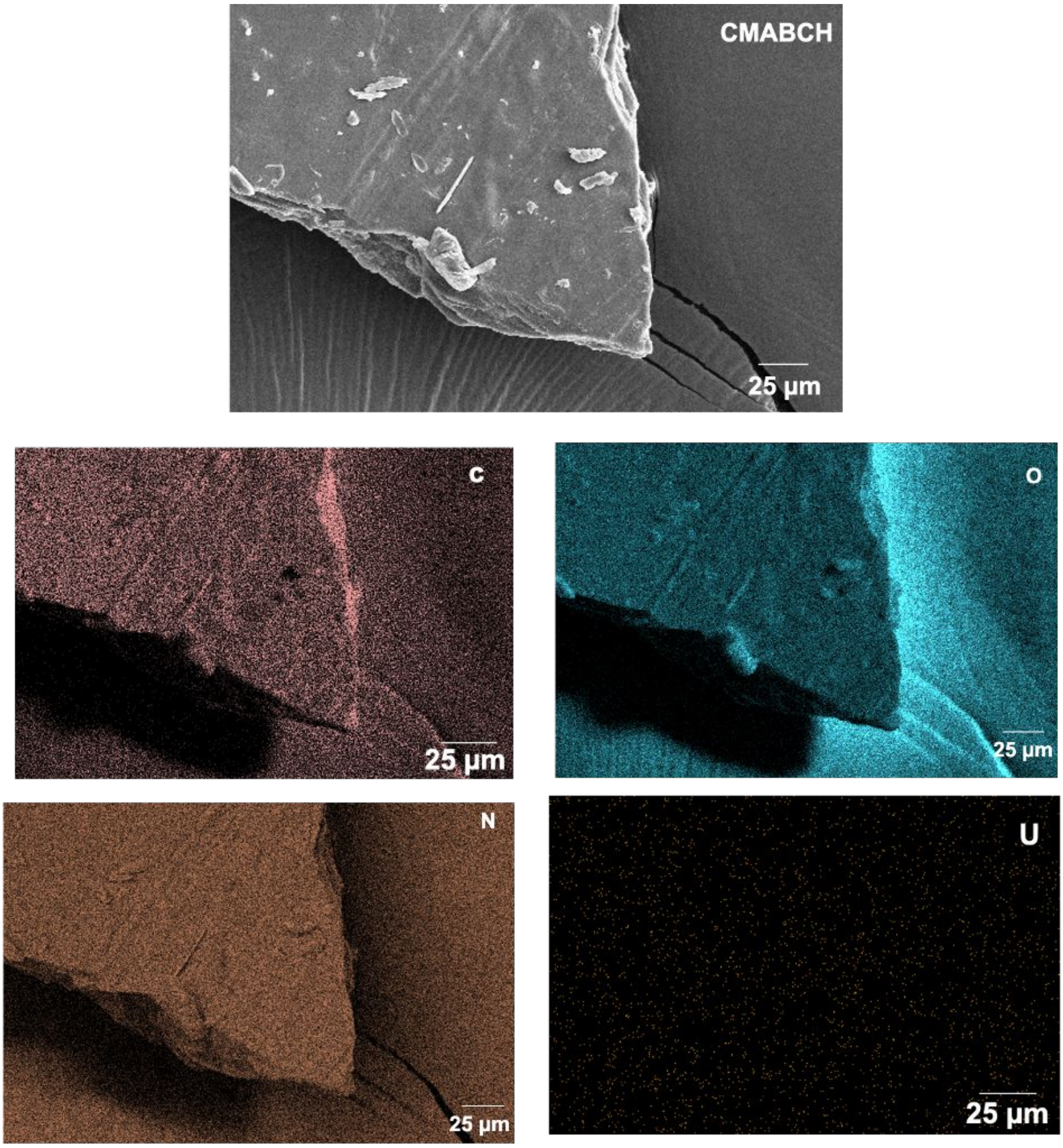

Figure S7. HRSEM image of CMABCH and its corresponding elemental mapping ($(U(VI))_o$-5000 mg/L, m-50 mg, V-10 mL, pH-7).

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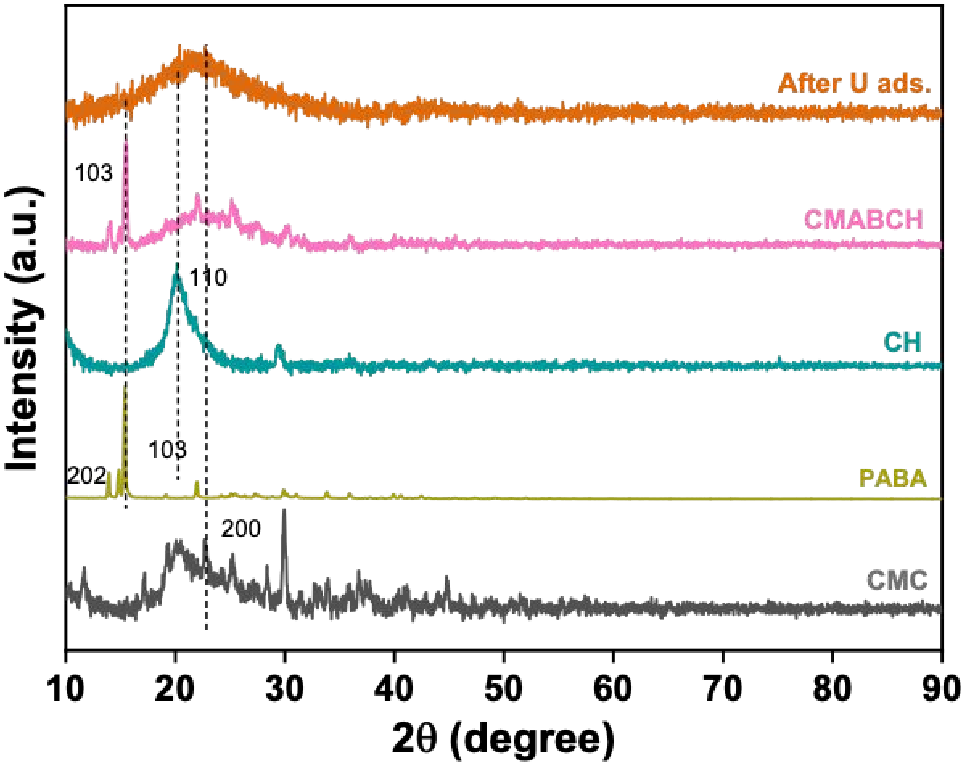

Figure S8. Powder XRD of CMABCH and its precursors, i.e. CMC, PABA and CH, and CMABCH after U(VI) adsorption ($(U(VI))_o$-5000 mg/L, m-50 mg, V-10 mL, pH-7).

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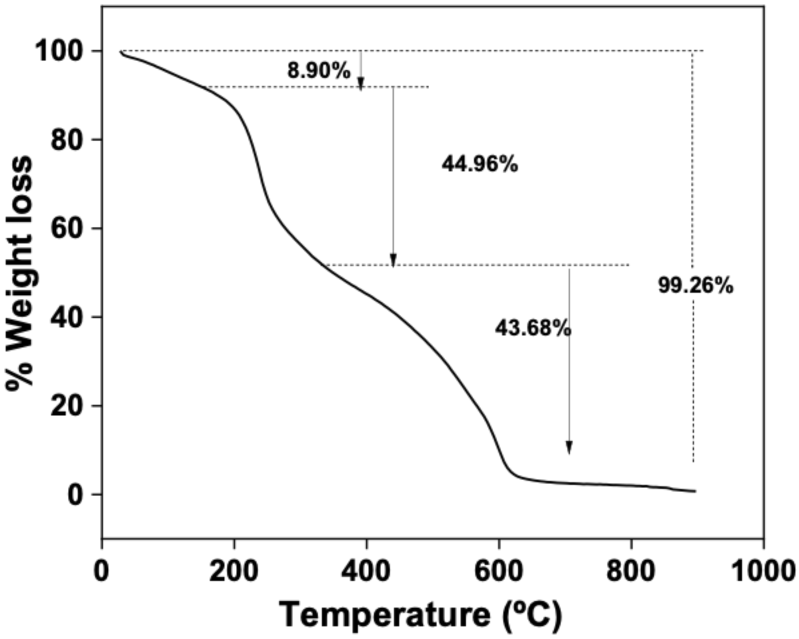
TGA in air



TGA in nitrogen

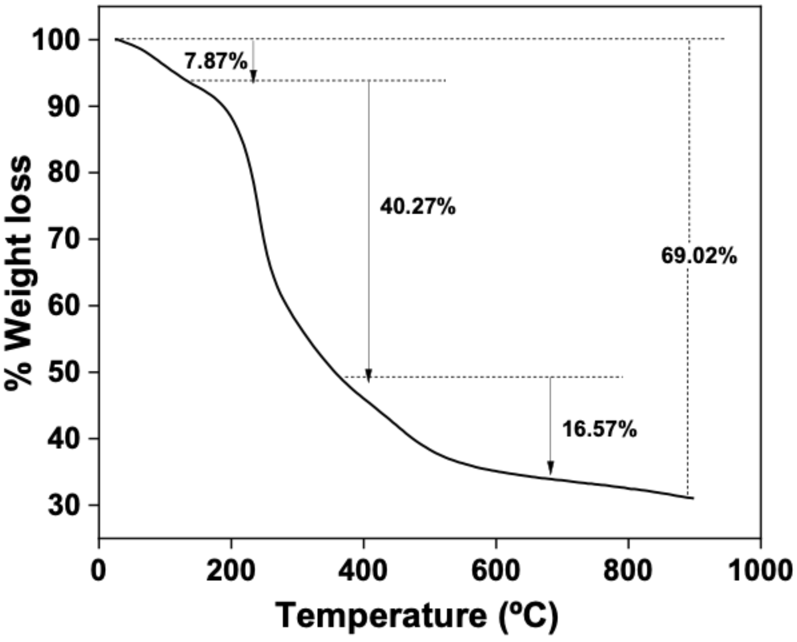


Figure S9. TGA of CMABCH in air and nitrogen atmospheres from room temperature to 900 °C at a scan rate of 5°C min^{-1}.

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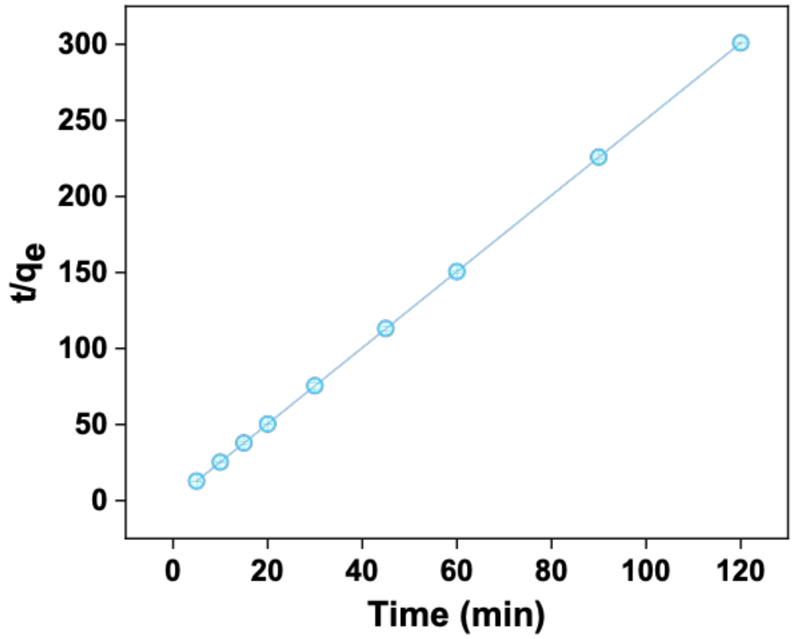

Figure S10. Ho's pseudo-second-order kinetic plot for the adsorption of U(VI) onto CMABCH, using eq S3.

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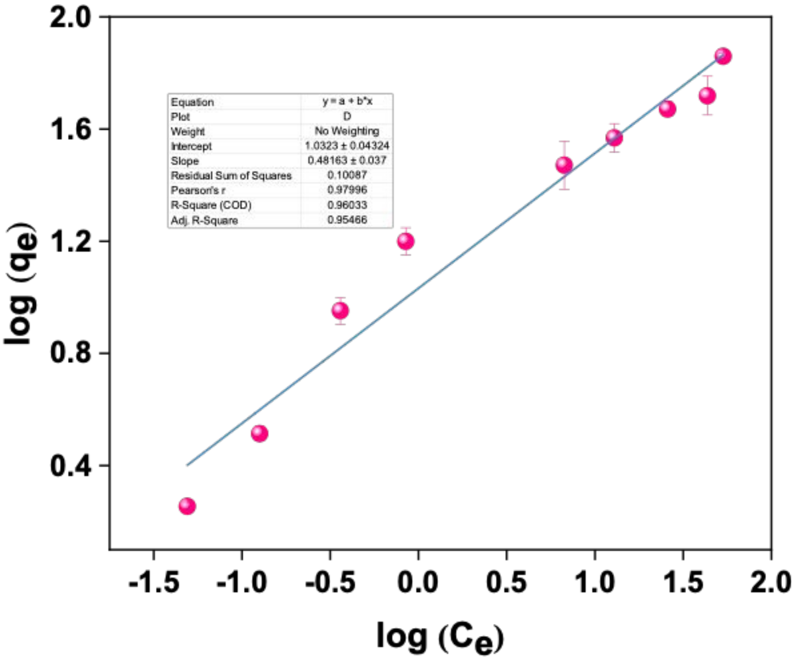

Equation	y = a + b*x
Plot	D
Weight	No Weighting
Intercept	1.0323 ± 0.04324
Slope	0.48163 ± 0.037
Residual Sum of Squares	0.10087
Pearson's r	0.97996
R-Square (COD)	0.96033
Adj. R-Square	0.95466

Figure S11. Freundlich isotherm plot for the adsorption of U(VI) on CMABCH using eq S5.

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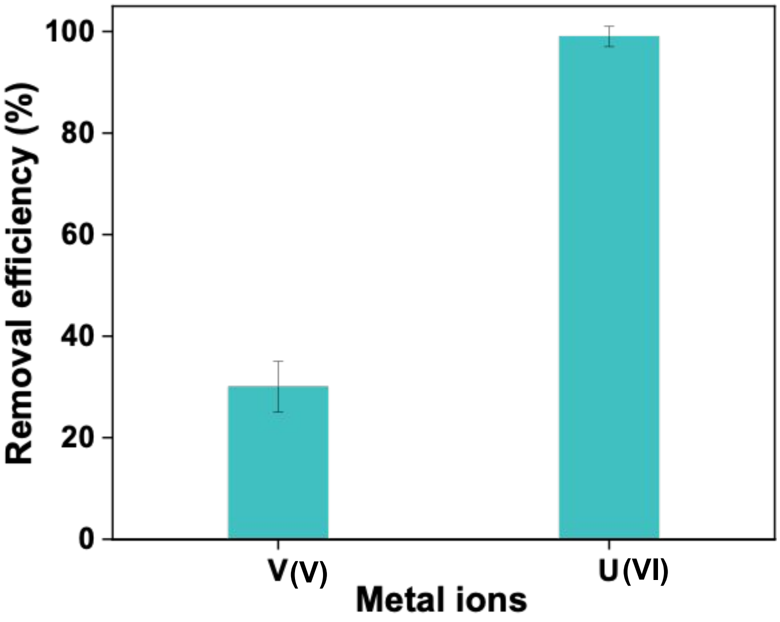

Figure S12. Removal efficiency of CMABCH when U(VI) and V(V) coexist U(VI)-1000 μg/L, V(V)-1000 μg/L, m-30 mg, V-10 mL, pH-7).

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Table S1: Desorption efficiency by various eluents

Eluents	Desorption efficiency (%)	Time (min)
HCl (100 mM)	**65**	**180**
HCl (50 mM)	**98.2**	**90**
HCl (10 mM)	**98.0**	**90**
Na_2CO_3 (100 mM)	**40**	**180**

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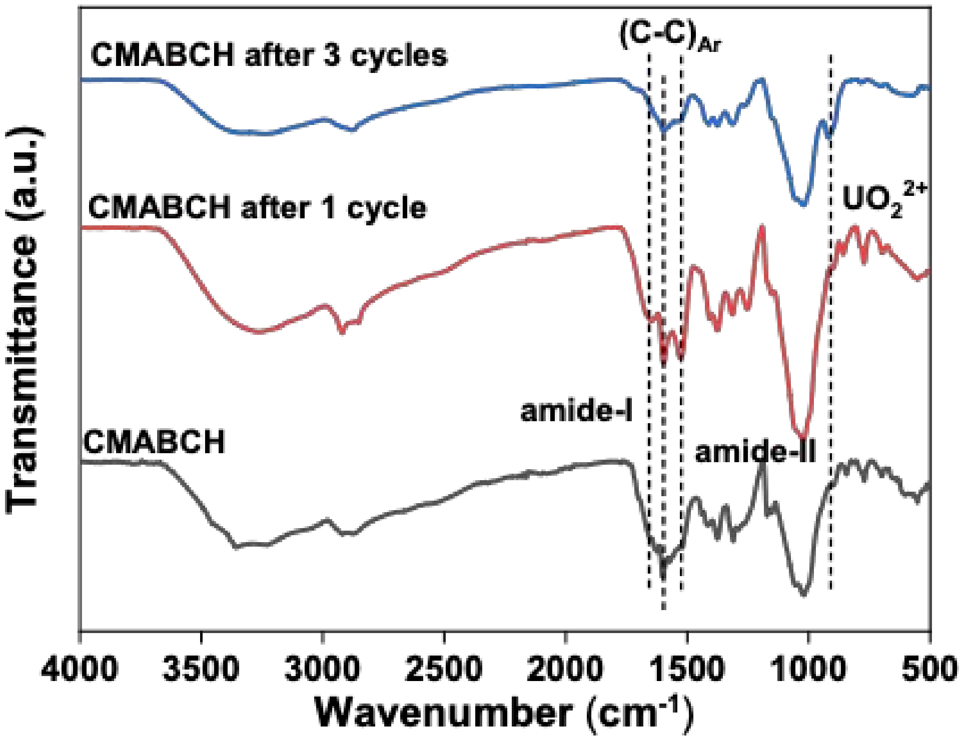

Figure S13. FTIR of CMABCH after adsorption-desorption cycles.

Table S2: Chemical parameters for the groundwater sample from the well in Shamshabad village, Fazilka, Punjab, India.

Parameter	Groundwater sample
TDS	663.5 mg/L
EC	2750 μS/cm
Turbidity	3.37 NTU
pH	8.5
Total alkalinity	240 mg/L
Mg^{2+}	16.72 mg/L
Ca^{2+}	6.45 mg/L
Li^{+}	4.76 mg/L
Ba^{2+}	0.043 mg/L
Sr^{2+}	0.504 mg/L
Mn^{2+}	0.417 mg/L
Pb^{2+}	0.0004 mg/L
Cd^{2+}	0.0001 mg/L
Ni^{2+}	0.0008 mg/L
U(VI)	0.102 mg/L
F^{-}	0.547 mg/L
Cl^{-}	134.6 mg/L
Br^{-}	0.684 mg/L
NO_3^{-}	0.709 mg/L
SO_4^{2-}	275.1 mg/L
PO_4^{3-}	Below detection limit