Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Title: Hydrophobic Core Formation and Secondary Structure Elements in Uranyl(VI)–Binding Peptides

Authors: Satoru Tsushima and Koichiro Takao

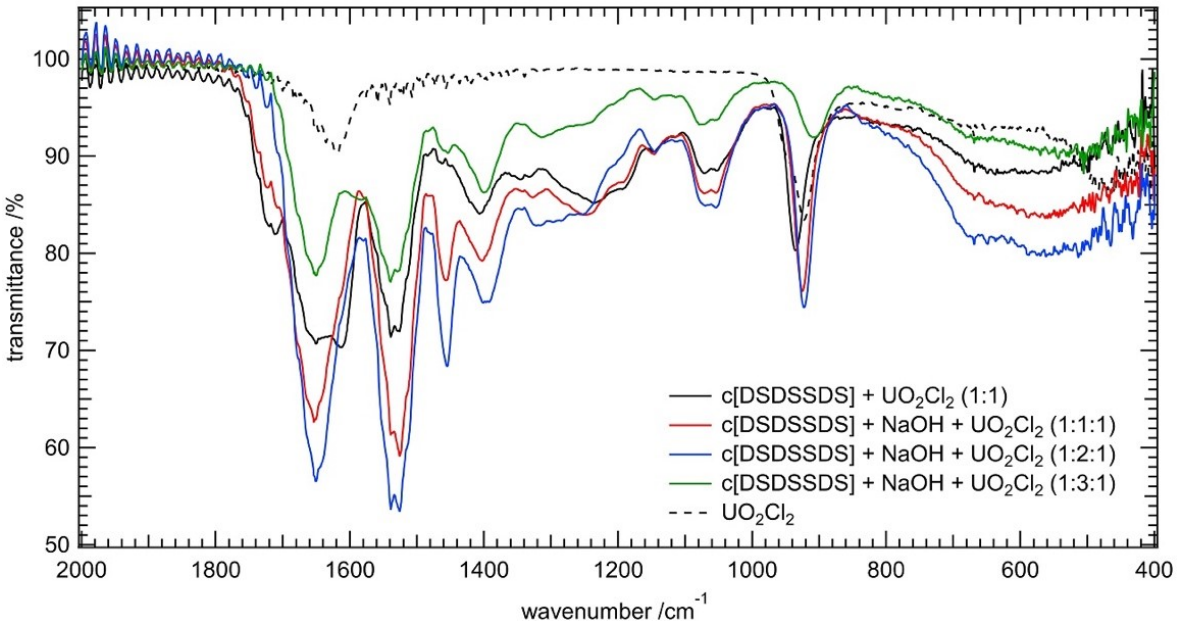

Fig. S1 FTIR-ATR spectra of c[DSDSSDS] in the presence of UO_2^{2+} with different amount of NaOH.

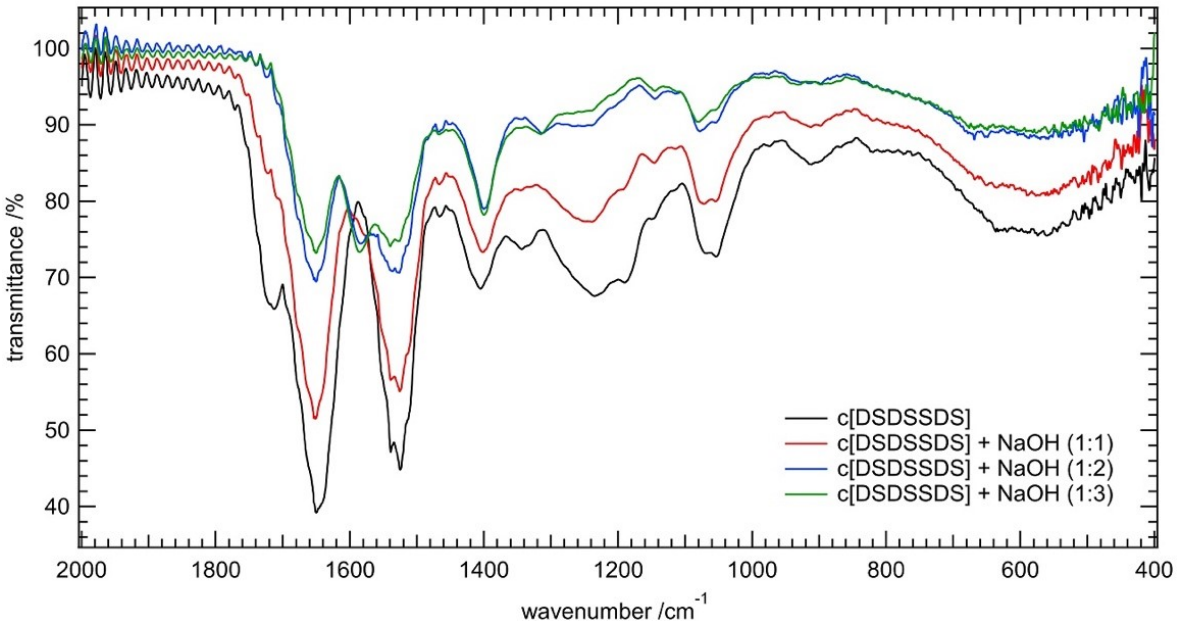

Fig. S2 FTIR-ATR spectra of c[DSDSSDS] in the absence of UO_2^{2+} with different amount of NaOH.

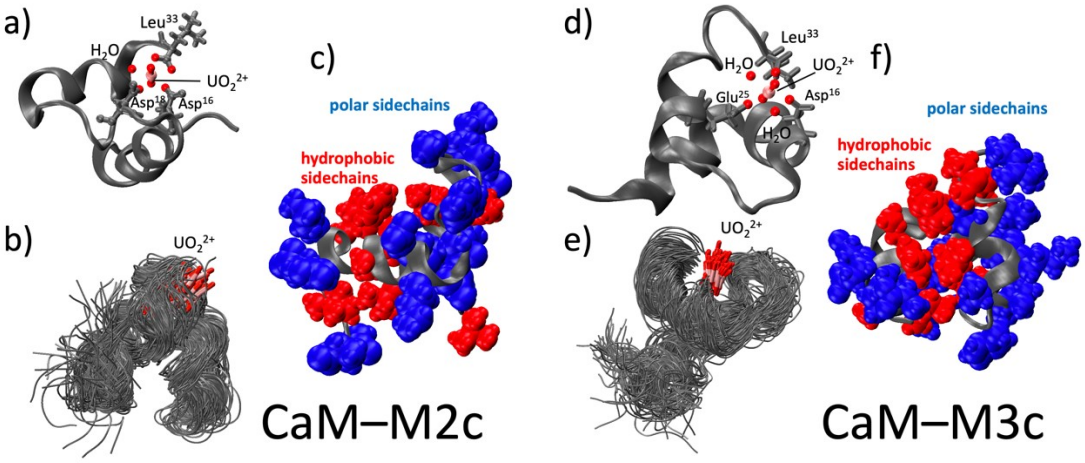

Fig. S3 Structures of UO_2^{2+}–bound CaM–M2c (a,b,c) and CaM–M3c (d,e,f) from the MD trajectories. Waters and Na^+ ions are omitted for clarity. (a,d): Global view on the peptide along the O=U=O axis from the MD snapshot at *t* = 200 ns. Peptide in dark ribbon, uranium in pink ball, oxygens in the vicinity of uranium in red balls. (b,e): Superpositions of 100 snapshots from 200 ns MD trajectory (each 2 ns). Peptide in gray ribbon and UO_2^{2+} in pink and red. (c,f): Global view on the peptide at *t* = 200 ns. Peptide in dark ribbon, hydrophobic sidechains in red, polar sidechains in blue spheres.

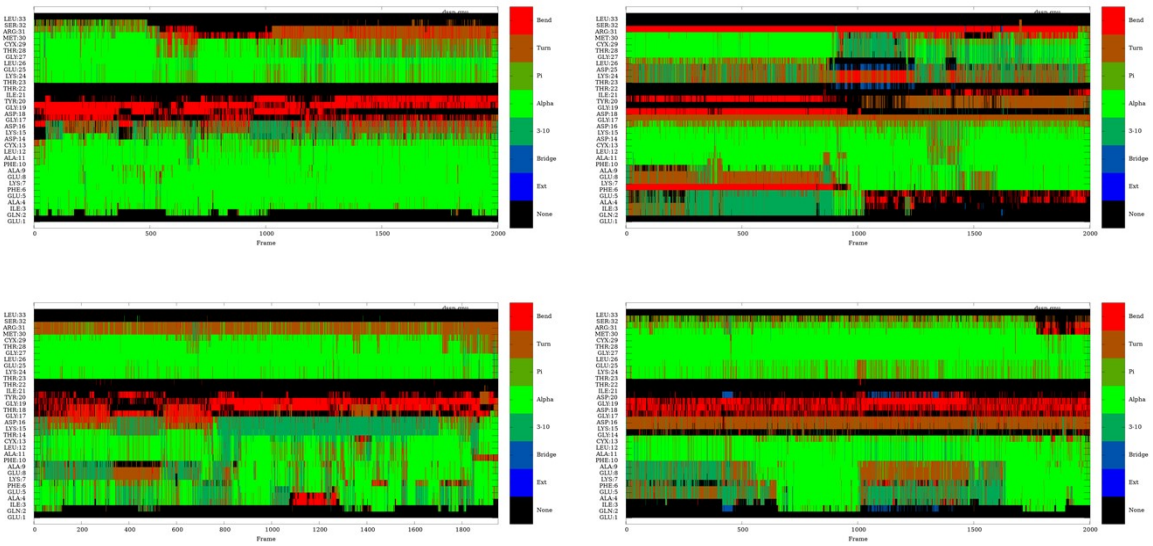

Fig. S4 Analysis of secondary structure elements of the UO_2^{2+}–bound CaM–M1c (top, left), CaM–M2c (top, right), CaM–M3c (bottom, left), and CaM-U2 (bottom, right) from the MD trajectories based on DSSP (hydrogen bond analysis algorithm).

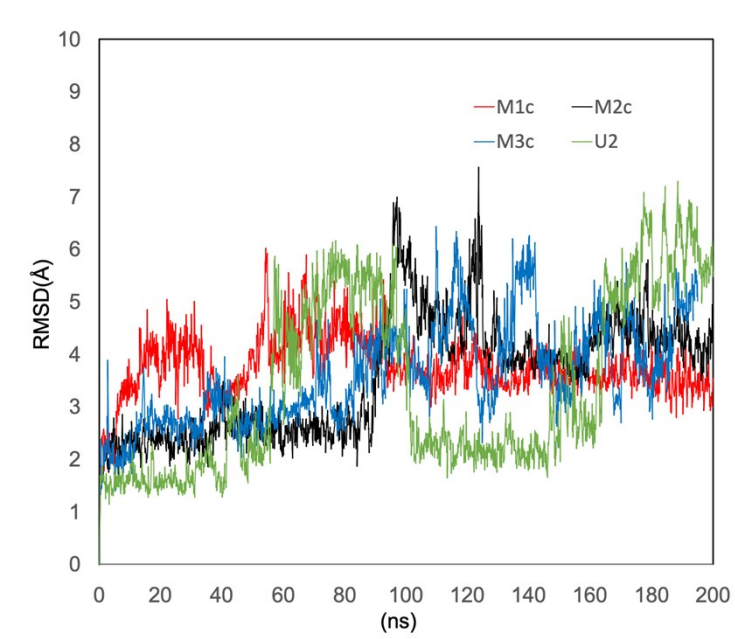

Fig. S5 Time evolution of RMSD of backbone atoms from 200 ns trajectories of MD simulations of CaM-M1c, CaM-M2c, CaM-M3c, and CaM-U2 with UO_2^{2+}.