Theoretical Studies on the Transport Mechanism of 5-Fluorouracil through Cyclic Peptide Based Nanotubes

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Electronic Supplementary Information:

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Figure S1: Model structures of \( \{\text{cyclo-}[\text{D-Trp-L-Leu}]_8 \} \) (a) and \( \{\text{cyclo-}[\text{L-Ala-D-Gln-L-Ala-D-Glu}]_2\text{-L-Ala-D-Gln}]_8 \} \) (b) system. The Leu and Ala amino acids are shown with ball and stick representation.
Figure S2: The spatial distribution function of 5FU during its transport through WL and QAEA systems. The amino acid side chains are not shown for clear visibility and the intermolecular H-bonding is represented as dotted lines.
Figure S3: Radial pair distribution functions g(r) between various atoms of 5FU and water H atoms of WL (A, B) and QAEA (C, D) systems. The densities as observed in the bulk water (A, C) and in the diffusion pathway (B, D).
Figure S4: The running average (window size 50) of number of H-bonds between water molecules and backbone carbonyl O atoms of various CPs from WL (A) and QAEA (B) systems as observed from the SMD simulation. The existence of van der Waals contact (with cut off distance of $< 3.5 \text{ Å}$) between 5FU and various CP units are represented with grey colour.
**Figure S5:** (a) van der Waals and (b) electrostatic energy contributions to the (c) free energy of binding of non H-bonded CPNT-5FU complex structures extracted from the SMD simulation of WL system.
Figure S6: (a) van der Waals and (b) electrostatic energy contributions to the (c) free energy of binding of non H-boned CPNT-5FU complex structures extracted from the SMD simulation of QAEA system.
Figure S7: Radial distribution function of water O around 5FU H₇/H₉ atoms in the presence of type A and B H-bonds observed from the WL (a) and QAEA (b) systems.
Figure S8: Water mediated H-bonds between CPNT amide N and various atoms of 5FU observed from the WL (A) and QAEA (B) systems. H-bonds: N(CPNT)···H–O(WAT)···N$_1$H$_7$(5FU) (black), N(CPNT)···H–O(WAT)···N$_3$H$_9$(5FU) (Green), N(CPNT)···H–O–H(WAT)···O$_8$(5FU) (Brown), N(CPNT)···H–O–H(WAT)···O$_{10}$(5FU) (Red).
Figure S9: Water mediated H-bonds between CPNT amide NH and various atoms of 5FU observed from the WL (A) and QAEA (B) systems. H-bonds: NH(CPNT)···O(WAT)···N1H7(5FU) (black), NH(CPNT)···O(WAT)···N3H9(5FU) (Green), NH(CPNT)···O–H(WAT)···O8(5FU) (Brown), NH(CPNT)···O–H(WAT)···O10(5FU) (Red).