Insight into molecular dynamics properties of gemcitabine anticancer drugs loaded inside an open-ended single-walled carbon nanotube

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Abstract

Single-walled carbon nanotube (SWCNT) is a successful candidate of a transporter in drug delivery system applications due to the unique characteristics such as high surface area and long cylindrical cavity. To investigate the behavior of loading multiple drug molecules encapsulated inside SWCNT, an anticancer drug gemcitabine varying in number from one to six molecules encapsulated inside a (18,0) open-ended SWCNT with 14 Å diameter and 34 Å length were investigated using classical molecular dynamics (MD) simulations. Throughout the simulation times of all systems, gemcitabine molecules always located inside the SWCNT due to the partial π-π stacking interaction between the aromatic cytosine ring of gemcitabine and the inner surface of the SWCNT, as well as the interaction among gemcitabine molecules themselves through the π-π stacking and hydrogen bond formation. At a low loading level (less than 21% w/v), the cytosine rings of adjacent drugs were likely to be orientated in a parallel-displaced conformation with a probable π-π interaction. In contrast, at high drug concentrations, the drug molecules are closer to each other inside the SWCNT and this apparently promotes their electrostatic interaction between gemcitabine molecules with multiple hydrogen bond formations, but they totally lose the π-π interaction between each other. These results suggest that the design of drug loading and releasing process for DDSs should take into account these types of intermolecular interactions in order to obtain a SWCNT-based DDS with a high capacity of drug loading and release processes.

References

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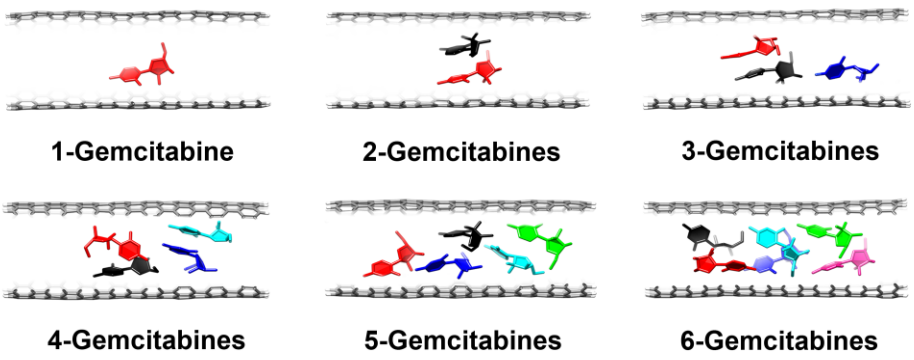

Figure 1 The representative structures taken from the last snapshot of six studied systems with different drug loadings contained inside the SWCNT cavity (1-6 gemcitabine molecules per SWCNT) are shown schematically.