

Supporting Information

Effect of temperature on the structure and drug-release behaviour of inclusion complex of β -cyclodextrin with cyclophosphamide: A molecular dynamics study

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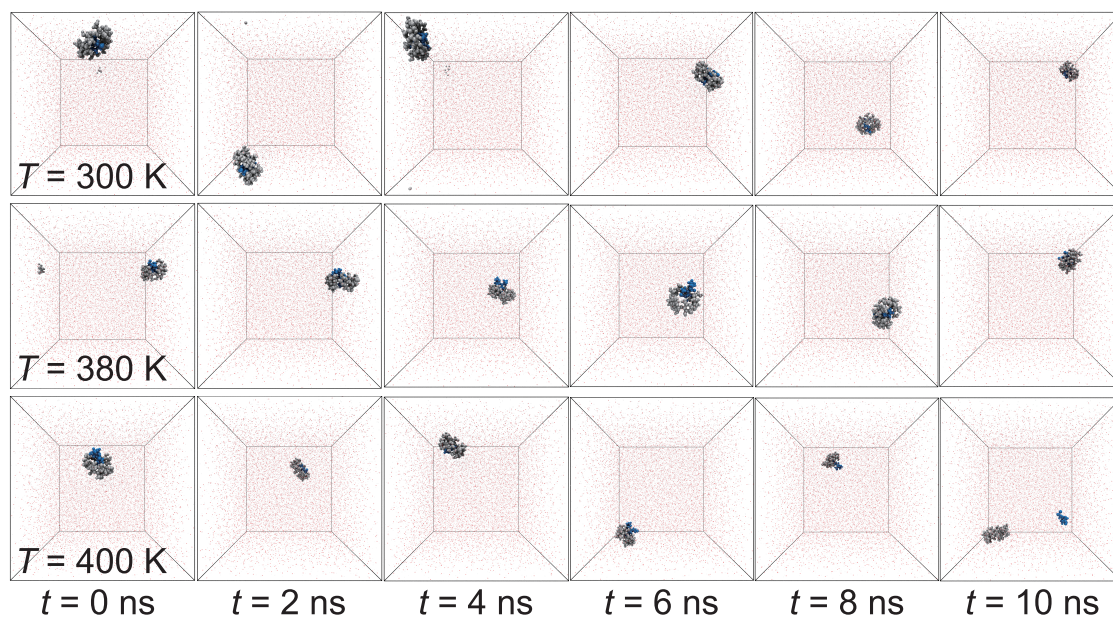


Figure S1 Representative simulation snapshots for the behaviours of the β -CD/CP complex and drug release.

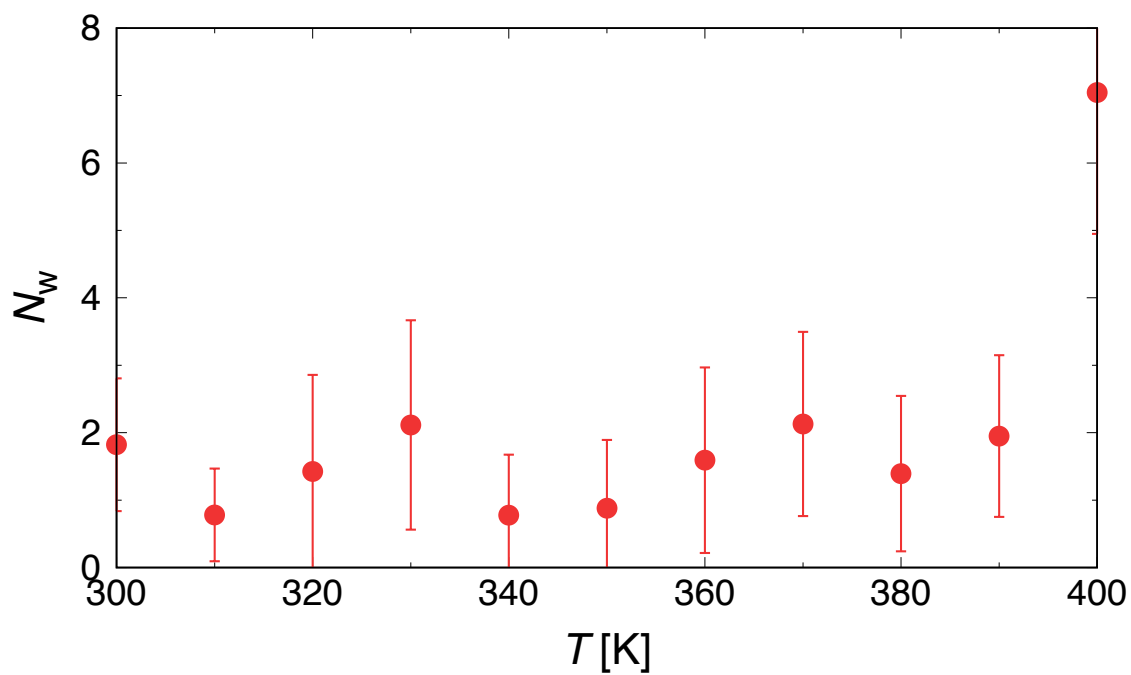


Figure S2 Average number of water molecules, N_w , in the β -CD cavity.

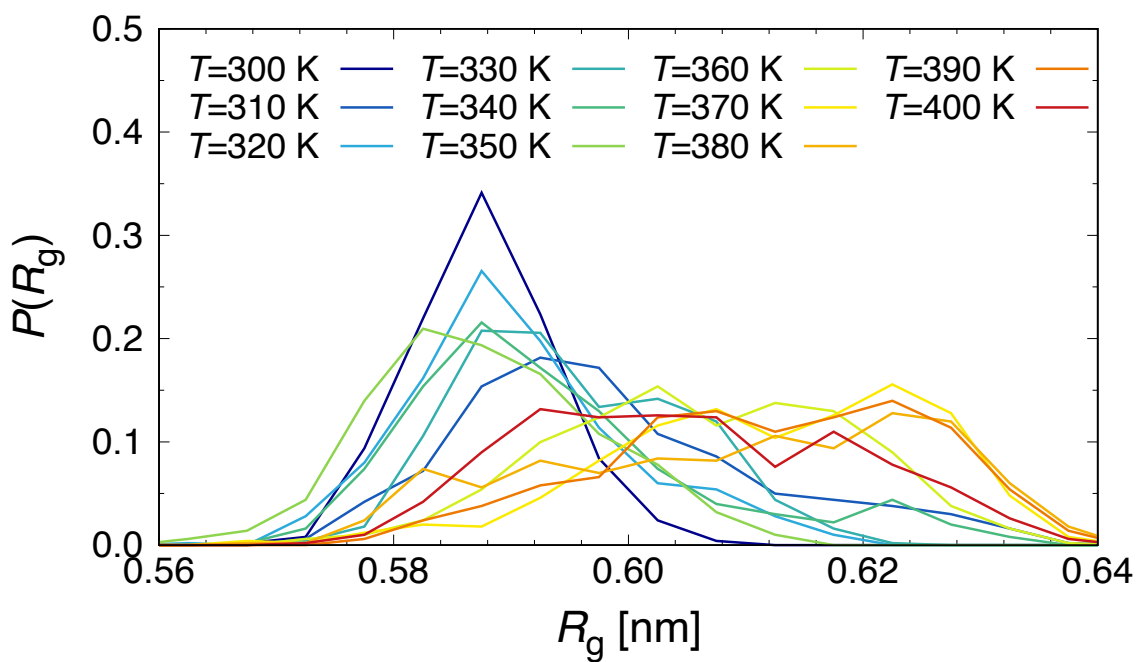


Figure S3 Probability distribution of the radius of gyration, R_g , of β -CD, $P(R_g)$ in the single-dispersion state for all investigated T , as indicated.