World Academy of Science, Engineering and Technology International Journal of Chemical and Materials Engineering Vol:18, No:08, 2024

Host-Assisted Delivery of a Model Drug to Genomic DNA: Key Information From Ultrafast Spectroscopy and in Silico Study

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Abstract : Drug delivery to a target without adverse effects is one of the major criteria for clinical use. Herein, we have made an attempt to explore the delivery efficacy of SDS surfactant in a monomer and micellar stage during the delivery of the model drug, Toluidine Blue (TB) from the micellar cavity to DNA. Molecular recognition of pre-micellar SDS encapsulated TB with DNA occurs at a rate constant of $k1 \sim 652 \text{ s}$ 1. However, no significant release of encapsulated TB at micellar concentration was observed within the experimental time frame. This originated from the higher binding affinity of TB towards the nanocavity of SDS at micellar concentration which does not allow the delivery of TB from the nano-cavity of SDS micelles to DNA. Thus, molecular recognition controls the extent of DNA recognition by TB which in turn modulates the rate of delivery of TB from SDS in a concentration-dependent manner.

Keywords: DNA, drug delivery, micelle, pre-micelle, SDS, toluidine blue

Conference Title: ICCST 2024: International Conference on Chemical Science and Technology

Conference Location : Venice, Italy **Conference Dates :** August 15-16, 2024