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Simulating the release of metformin as anti-diabetic drug from carbon nanotubes

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Diabetes mellitus (DM) and its complications constitute a serious public health issue facing modern societies (1). Metformin is currently the most widely used hypoglycemic drug for diabetes mellitus (2). Furthermore, in recent years, it has been determined that, this drug has direct effects on cancer cells.

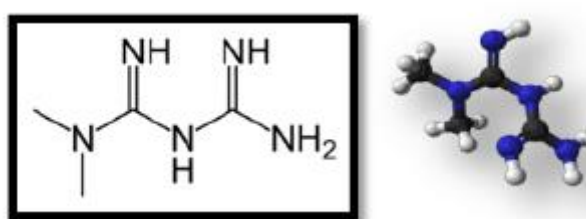


Fig. 1: Structure of N,N-Dimethylimidodicarbonimidicdiamide (Metformin)

Based on previous research, it was demonstrated that metformin loaded on carbon nanotubes under near-infrared (NIR) irradiation led to a significantly increased response to cancerous cells. Molecular dynamics simulations are a very powerful method to Study the drug delivery process and improve its efficacy and safety by controlling the rate, time, and place of release of drugs. in this study the dynamic release of metformin from the interior of carbon nanotube in the aquatic environment using the dl-poly software.

Keywords: Diabetes, Diabetes mellitus, Metformin, Molecular dynamics simulation

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