

IMPROVING THE EFFICACY OF AMINE CONTAINING MEDICINES: A COMPUTATIONAL APPROACH

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In this computational study, approximately 150 well known medicinal agents, from malaria drugs to cancer treatments, are examined as candidates for improving their efficacy by increasing their water solubility. Each of these agents have a similarity, they contain an amine. As opposed to other approaches such as liposomes and other micelle approaches, nanoparticles and proteins, this presentation will show that a number of drugs can have improved water solubility and hence better treatment efficiency by binding the amine structure to a specific cation in the correct molecular location. The ratio of the molecules dipole moment (D ; Debye) to molecular volume (V , Å^3) or its D/V ratio when unbound compared to the bound complex is used to make the physiological argument.