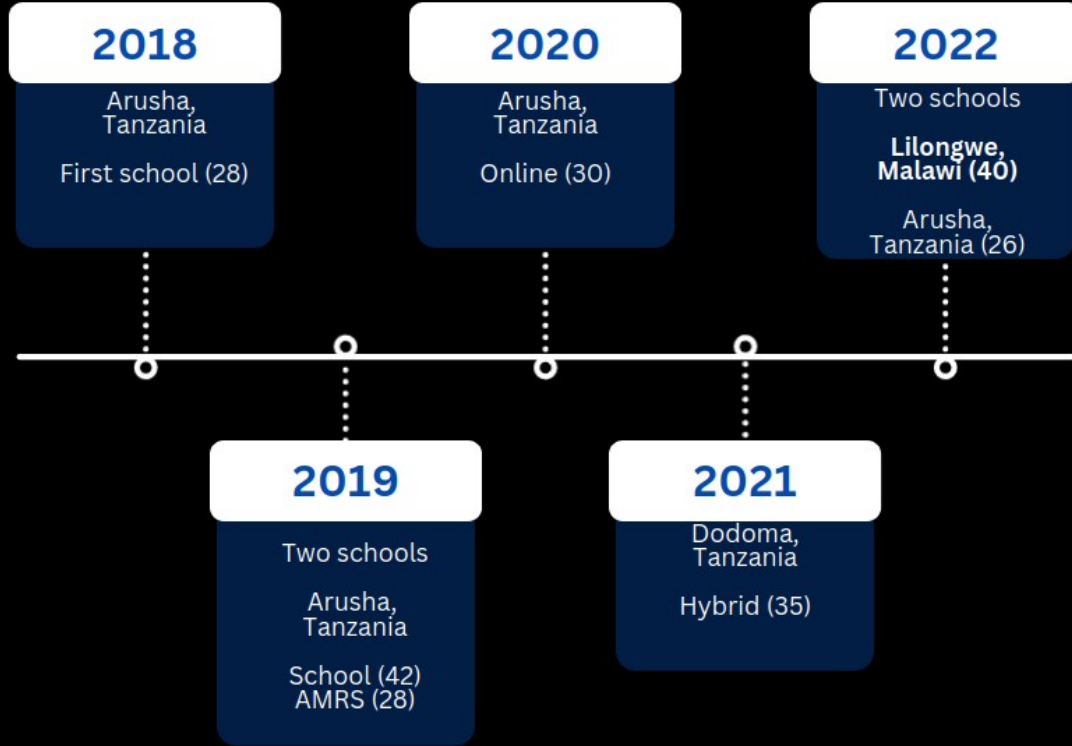


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Previous years



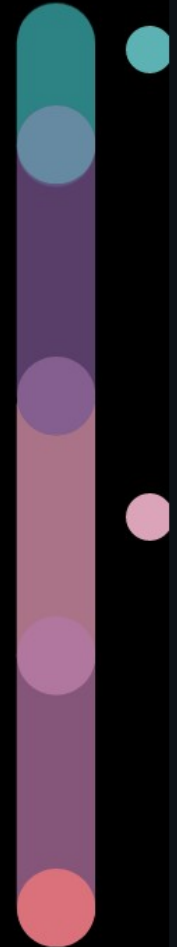
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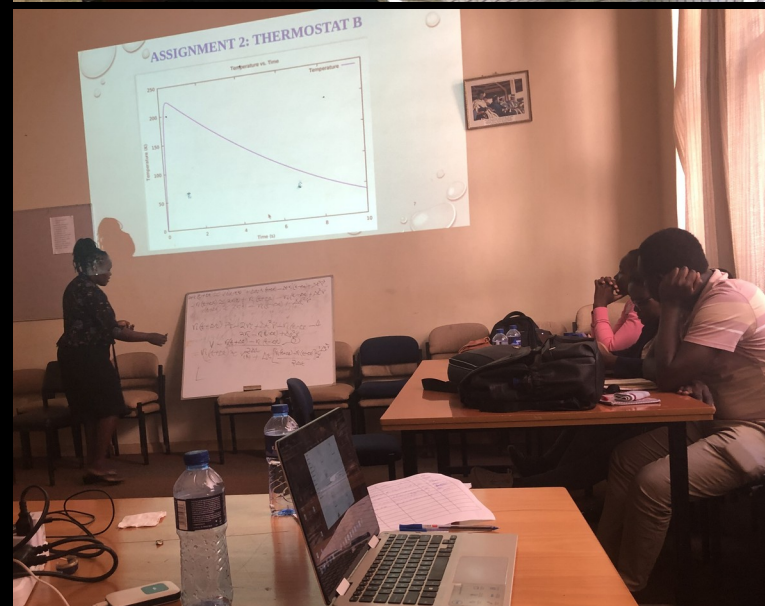
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Investigation of the structure, stability, and relative solubility of psilocybin in water and pure organic solvents: A molecular simulation study

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ABSTRACT

Psilocybin is an indole-based secondary metabolite found naturally in mushrooms which possesses several pharmacological effects. Recently, a large number of experimental investigations have been conducted to characterize the pharmacology of psilocybin and its derivatives, and to develop synthetic pathways to manufacture psilocybin. Nonetheless, current research on the physical characterization of psilocybin is limited in part due to legal restrictions. In the present study, we investigate two unique tautomers of psilocybin as depicted in the 2D chemical structure of psilocybin presented in the recent literature. Using a combination of electronic structure calculations and molecular simulation, we are able to identify and characterize the thermodynamically

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