INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study	:	Ph.D.

Thesis Title: “The Role of Aggregation of Melamine and Uric Acid in Kidney Stone Formation and its Inhibition by Small-Molecule Inhibitors in Solution and at the Solid-Liquid Interface: A Computational Approach”

Name of Thesis Supervisor(s)	:	Prof. Sandip Paul
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The thesis focuses on the aggregation property of small molecules related to various diseases that occur in humans and their inhibition by applying drugs with the use of molecular dynamics simulation in the solution phase and solid-liquid interface. Thus far, the research findings are very enlightening. In this thesis, we have found an imperative conclusion that the aggregation propensity of uric acid is higher than uric acid-melamine and melamine-melamine interactions; consequently, a large cluster of uric acid molecules results. Such large clusters (comprised of uric acid) "drag" neighbouring melamine molecules towards themselves to add to it, and thereby an insoluble melamine-uric acid cluster is produced. The significance melamine-uric acid aggregation is that these interactions are responsible for forming melamine-induced kidney stones in humans. Therefore, if one needs to break the melamine-uric acid interaction, either the interruption of the pi-stacking among uric acid molecules or the inhibition of melamine-uric acid hydrogen bonding interaction is necessary. Moreover, we have employed various small molecule inhibitors like theobromine, allopurinol, potassium citrate, and vitamin C to inhibit their aggregation inthe solution and a solid-liquid interface to prevent the kidney stone.