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Effects of spermine binding on Taxol-stabilized microtubules

SHENGFENG CHENG, CHOLA REGMI, Virginia Polytechnic Institute and State University — Previous studies have shown that polyamines such as spermine present in cells at physiological concentrations can facilitate the polymerization of tubulins into microtubules (MTs). A recent experiment demonstrates that in the presence of high-concentration spermine, Taxol-stabilized MTs undergo a shape transformation into inverted tubulin tubules (ITTs), the outside surface of which corresponds to the inside surface of a regular MT. However, the molecular mechanism underlying the shape transformation of MTs into ITTs is unclear. We perform all atom molecular dynamics simulations on Taxol-stabilized MT sheets containing two protofilaments surrounded by spermine ions. The spermine concentration is varied from 0 to 25mM to match the range probed experimentally. We identify important spermine binding regions on the MT surface and the influence of the spermine binding on the structure and dynamics of MTs. In contrast to Taxol, our results show that spermine binding seems to decrease the flexibility of tubulin proteins, resulting in weaker tubulin-tubulin contacts and promoting the bending of protofilaments into curved protofilaments, inverted rings, and eventually inverted tubules.

Shengfeng Cheng
Virginia Polytechnic Institute and State University

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