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Targeting microtubules in cancer research: Application of computational simulations in developing novel chemotherapeutic agents

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Microtubules (MTs) with a cylindrical shape are essential functional elements in all eukaryotic cells and are formed by polymerization of tubulin-heterodimers. The mechanism of unequal segregation of chromosomes has shown correlations with tumor development and birth defects. Since MTs dynamics facilitate the arrest of cell division in the G2-M phase of the cell cycle, they have been a popular target in cancer research. In the presented work, using computational molecular modeling methodologies, the currently in use cancer drugs are studied. The *in silico* techniques are employed to explain drugs binding site, their mode of action and mechanism of their involvements with MTs assembly when complexed with the heterodimer. These data lead to identification of key interacting fragments of the drugs, the involving components of the heterodimer, and the short- and long-range impacts of the drugs on folding patterns of the protein segments which are linked to MTs polymerization/depolymerization process. Moreover, the results are implemented for target-based design of novel lead compounds and development of new generation of chemotherapeutic MT-agents with high anti-tumor activities and minimum toxicity.

Biography

Laleh Alisaraie has completed her Ph.D. in Natural Sciences from Universität Paderborn in Germany and Postdoctoral studies in Computational Structural Biology at McGill University. She is an Assistant Professor of Pharmaceutical Sciences at the School of Pharmacy in Memorial University of Newfoundland and Labrador in Canada. Alisaraie's research area includes computational medicinal chemistry and *in silico* drug design as well as structure and function of multi-component biochemical complexes, protein folding, processing and degradation.

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