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Title: A radical approach to enhance students' involvement in undergraduate research: Insights into computational methods for targeted antitumor drug discovery against HDACs

Abstract

Conducting academic research is a pivotal strategy to enhance healthcare students' critical thinking and problem-solving skills, which improve their performance in clinical practice (1). According to previous reports, financial difficulties and lack of research topics are two prominent obstacles preventing students from engaging in undergraduate research (2, 3). Therefore, this literature review could offer an accessible pathway for students' involvement in research since the computer-aided approaches typically require reduced time and cost (4). Profound understanding of medical terms, particularly cancer pathology and targeted antitumor treatments, potentially assists researchers in the development of effective therapies. This review centers on HDACs (histone deacetylases) and recent applications of in silico tools in the discovery of therapeutic drugs for cancer treatment as promising subjects of medical research. HDACs are a group of enzymes that accelerate the removal of acetyl groups from lysine residues on histones and thus lead to chromatin condensation (5). Overexpression of HDACs, contributing to the initiation of various types of cancer, has been indicated in previous works (6, 7). HDACs have been considered as potential targets for anticancer drugs; consequently, HDAC inhibitors have emerged as novel oncological treatments by targeting the active sites of these enzymes (7, 8). Simulation-assisted methods, including molecular docking and molecular dynamics, have been utilized to enhance the discovery of HDAC inhibitors (9, 10). Rational design of HDAC inhibitors, significantly supported by computer-based methods, could serve as innovative approaches for undergraduate studies. By providing feasible research ideas and cost-effective computational strategies, these outcomes might help students overcome commonplace hurdles such as limited research subjects and insufficient funds while encouraging them to develop essential skills for patient care.

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