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Using Computer-Aided Drug Design (CADD) techniques to optimize the natural product-derived phenylmethylidene-hydanto in scaffolds as promising antimetastatic leads

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Prostate and breast cancer is the second most prevalent cause of mortality in men and women, respectively. Approximately one-half of the current anticancer medications have been originally derived from natural products. Although a natural product can directly functionas a lead compound, considerable refinement in the natural product's chemical scaffold is typically required to optimize the product's pharmacodynamic factors. These factors include, but are not limited to, binding affinity, drug-likeness, cLogP, LogS, molecular weight, and an overall risk for toxicity. The optimization process accentuates the compound's intrinsic potential to qualify as a lead candidate. Computer-aided drug design (CADD) techniques are widely used in natural product research to accelerate the process of overall drug design and discovery. This presentation will illustrate a proof-of-concept of this process using the example of 4 (hydroxyphenylmethylidene) hydantoin (PMH), (5Z)-5-(4-hydroxybenzylidene) imidazolidine-2, 4-dione. This chemical entity is a natural product isolated from the Red Sea sponge *Hemimycale Arabica.* This product has demonstrated antimetastatic activity in a number of in vitro/ *in vivo* models of prostate and breast cancer. Based on the natural product inspired scaffold, several related analogs of PMHs were synthesized to improve the antimetastatic activity. This talk will present the various CADD techniques that were usedto optimize PMH activity. This optimization resulted in severalfold-improvementin the *in vitro/in vivo* antimetastatic properties. This presentation will underscore the importance of computer-aided design in natural product research and its application in improving the efficiency of the drug discovery and development process.

Biography

Mudit Mudit joined D'Youville College as an Assistant Professor in the School of Pharmacy's Department of Pharmaceutical, Social and Administrative Sciences in Fall 2010. He earned his PhD in Pharmaceutical Sciences from the University of Louisiana at Monroe (ULM). He is an active member of several professional organizations including the American Association of Colleges of Pharmacy (AACP), American Association of Pharmaceutical Scientists (AAPS), American Chemical Society (ACS), and Kappa Psi Pharmaceutical Fraternity. He has given numerous research presentations both at regional and national meetings, and has been recognized by the AAPS for excellence in graduate education in the fields of Drug Design and Discovery (DDD).

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