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### ***“Computer-Aided Molecular Design: Approaches and Applications”***

Computer-aided molecular design (CAMD) is a cost-effective technique which allows researchers to computationally generate molecular structures according to an algorithm and score those structures for fitness. While CAMD has had notable achievements in the drug design area, it is also used in the chemical process industry. In this presentation, I will provide background on some of the basic CAMD techniques and successes. Additionally, I will focus on one such technique using the Signature molecular descriptor. We will show that Signature possesses desirable features (relative to other descriptors) which make it well-suited for a CAMD approach. Applications to the design of ICAM-1 inhibitors will be presented as well as other studies using this approach, including solvent design and ionic liquids as biomass pretreatment options.