Development and Implementation of Websites and Web Applications for a Blended Organic Chemistry Course

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Chemistry on the World Wide Web (WWW) has come into its own in recent years with the blossoming of computational chemistry and chemoinformatics. In many ways, the maturity of these fields has fundamentally altered how practicing organic chemists approach problem solving and experimentation. However, despite this progress, chemical educators have been relatively slow to embrace computational chemistry and chemoinformatics software.

For a blended organic chemistry course, we have designed, developed, and implemented a wide variety of websites and web applications that take advantage of software and algorithms for computational chemistry and chemoinformatics. Our experience has shown that these tools promote significant learning provided certain conditions are met. A focus on usability during the design stage and sufficient guidance for students at all levels of technical expertise are essential. Continuous development based on student feedback is a third critical idea, which we have used to regularly refine and improve our software. By embracing chemoinformatics and computational chemistry, we have been able to replace outmoded algorithmic problems with those aimed at developing sound chemical reasoning skills.

Construction of Stereochemically Complex and Structurally Diverse Compounds from Quinine

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High throughput screening is the dominant method for pharmaceutical lead discovery, yet most screening collections consist of planar molecules that lack the structural complexity necessary for the modulation of numerous drug targets. To address this deficiency, we have developed a novel, general, and facile approach for the rapid generation of complex and diverse small molecules. Starting from readily available complex natural products, structural diversity is achieved through the strategic manipulation of core ring systems. To demonstrate this approach, short synthetic sequences of ≤5 steps have been used to transform the *Cinchona* alkaloid natural product quinine into five molecular scaffolds that are strikingly different from each other and the parent natural product.