Drug discovery through integration of synthetic organic chemistry and computational chemistry: how can I make better use of computational chemistry?

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Historically, the development of new drugs has been achieved through close coordination between conventional synthetic organic chemistry and biology (pharmacology), in which new drugs were created much like hand-crafted products. On the other hand, recent rapid progress in genome science and information technology, along with new technologies such as combinatorial chemistry, high-throughput screening, computer-aided drug design, and *in silico* screening have had a major impact on research for new drug development. Obviously, for more efficient discovery of lead compounds and their optimization, the integration of these new technologies and conventional approaches is necessary. However, does the typical synthetic organic chemist truly understand and make good use of data derived from computational chemistry or structural biology obtained using rapidly advancing computer science? This lecture will give the impressions and expectations of computational chemistry from the perspective of a present-day synthetic medicinal chemist.