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The Beauty of Computational Drug Design

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Abstract

Breast cancer cells are spread to new locations in the body via metastasis. Inflammatory cytokines play an important role in mediating this process, and thus provide a promising target for preventive research. Our research focuses around testing and synthesizing new small molecule inhibitors (SMIs) to inhibit a specific inflammatory cytokine in the breast cancer metastasis. An important part of drug discovery is the *in silico* drug screening via molecular dynamics simulations. Leveraging the computational resources on campus we can estimate the binding affinity of a drug candidate to an inflammatory cytokine, helping identify the most promising candidates for synthesis and further testing. The image presented here is a snapshot from one of these simulations.