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Experimental and Computational Study of Beta-Galactosidase Inhibition ANTHONY COOPER, LUCA LARINI, Rutgers University-Camden — In this study, we combine experiments and simulations to design novel inhibitors of enzymes. We aim to characterize the inhibition mechanism which we show to be dependent on the aggregation of inhibitor peptides. As a model system we chose to use β-galactosidase. We selected four peptides out of 10,000 initially screened using microarrays and that show the greatest Michaelis-Menten constant and highest solubility. Molecular dynamics simulations were performed to identify the exact mechanism of action of these peptides. We show that the positive residues, like arginine and lysine, are crucial for inhibiting enzyme activity. According to simulations, these residues are also responsible for the conformations adopted by the peptide in solution. Dynamic light scattering study revealed that the aggregation of peptides with the enzyme takes place and is responsible for inhibiting enzyme activity.

Anthony Cooper
Rutgers University-Camden

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