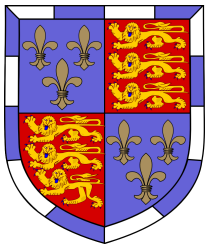
Developing a computational pipeline to determine optimal affibody scaffold positioning



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This dissertation is submitted for the degree of
Master of Science

St. John's College

April 2024

Abstract

We present a method for positioning Affibody scaffolds, conditioned on a target structure, that serves as a starting point for the computational design process of Affibodies binding to said target. Our method utilises the LightDock docking framework combined with a flexible, distance-based scoring function which is agnostic of the identity of the variable residues on the Affibody binding surface. When provided with the 'ground-truth' epitopes of 8 experimentally determined Affibody complexes, our docking pipeline showed a mean RMSD of 2.95 ± 1.8 Å for the top scoring structure, producing backbone models which are within the desired RMSD to be used as an input for a sequence design and local structure refinement deep learning framework currently under development in our group.