Data-driven Support System for Computer-Aided Antibody Design

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Introduction

- Antibodies are crucial for therapeutics, diagnostics, and research.
- Traditional antibody production is expensive, time-consuming, and ethically challenging.
- Computational antibody design offers a sustainable, cost-effective alternative.
- This project aims to develop an end-to-end computational pipeline for antibody design.

Problem Statement

- Traditional methods rely on animal immunization, leading to batch-to-batch variation.
- High costs and ethical concerns associated with animal use.
- Lack of an automated, data-driven tool for antibody design.
- Need for a user-friendly, general-purpose antibody design pipeline.

Objectives

- Develop computational methods for antibody design (Aim 1).
- Integrate these methods into a user-friendly web-based tool (Aim 2).
- Validate computationally designed antibodies through *in vitro* assays (Aim 3).

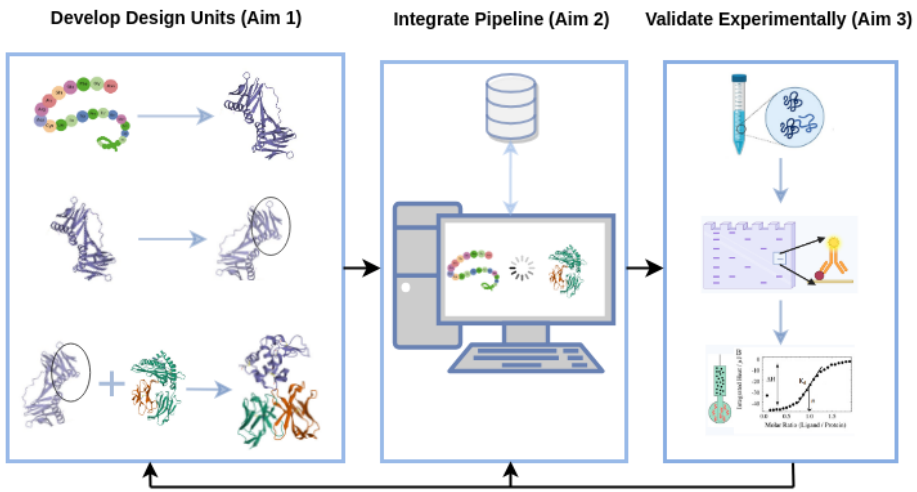

Figure: Overall workflow of the computational antibody design pipeline.

Workflow

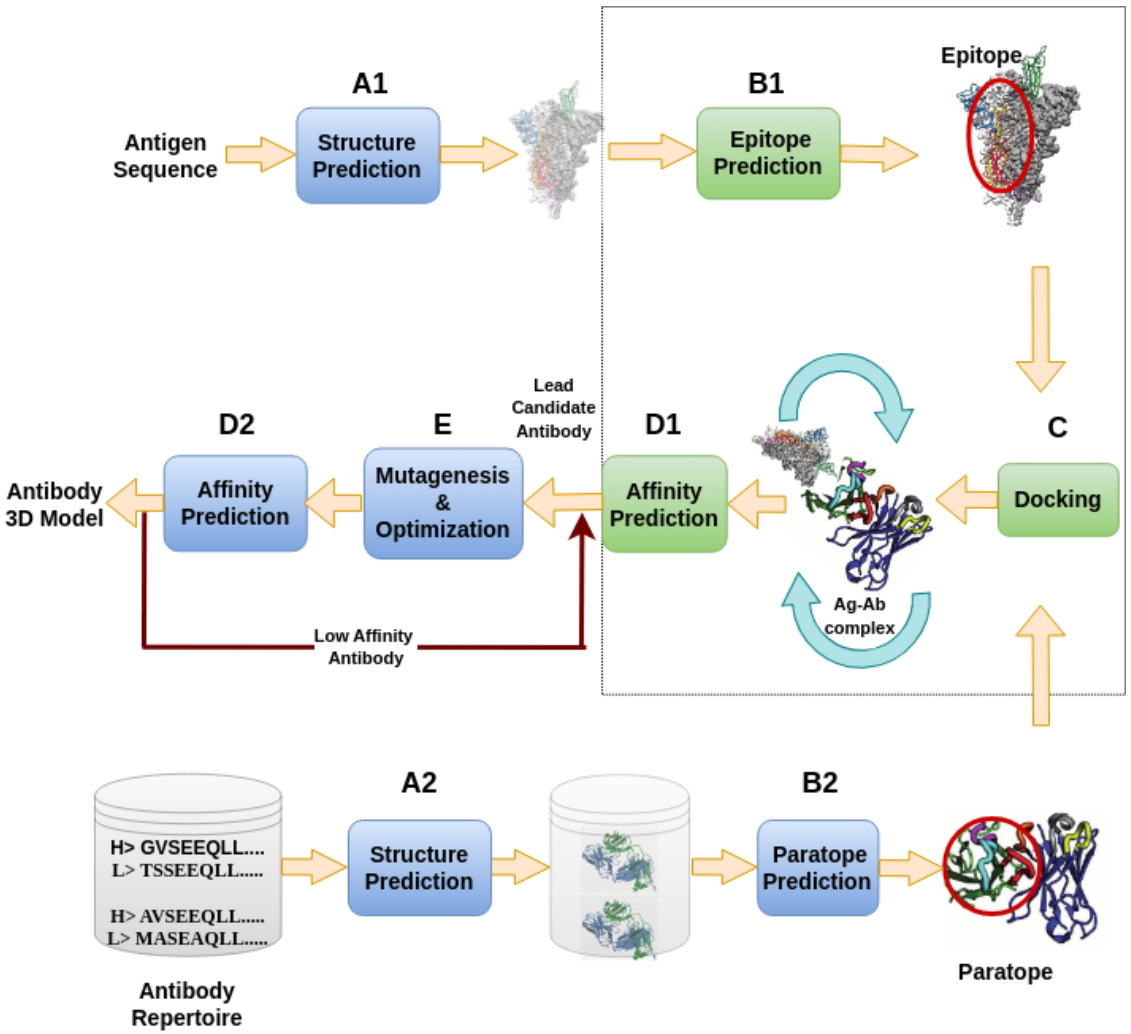

Figure: Overall workflow of the computational antibody design pipeline.

Aim 1: Computational Methods

- Predict 3D structures of antigens and antibodies.
- Predict binding sites (epitope and paratope).
- Perform antigen-antibody docking.
- Predict binding affinity and optimize energy through mutagenesis.

Aim 2: Integration and Deployment

- Develop a user-friendly web-based tool.
- Integrate computational methods into an end-to-end pipeline.
- Provide a graphical interface for researchers and industry professionals.

Aim 3: In Vitro Validation

- Validate computationally designed antibodies using:
  - Immunoblot assays.
  - Isothermal titration calorimetry (ITC).
  - Immunofluorescence microscopy.
- Compare results with commercially available antibodies.

Aim 3: Wetlab Validation Workflow

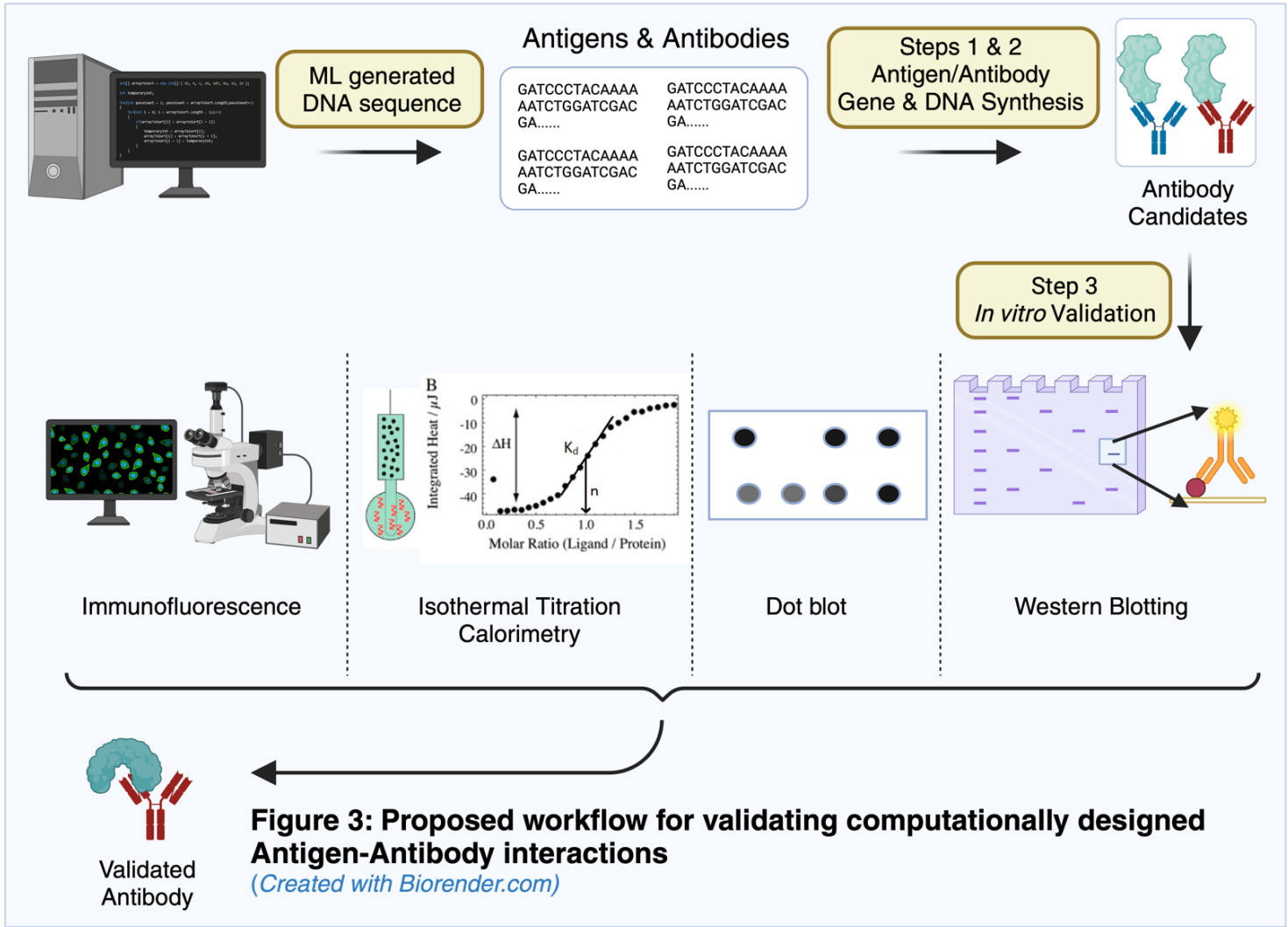

Figure 3: Proposed workflow for validating computationally designed Antigen-Antibody interactions
(Created with Biorender.com)

Figure: Wetlab validation workflow for antibody testing.

Significance

- Revolutionize antibody design by reducing time and cost.
- Eliminate ethical concerns associated with animal use.
- Provide a sustainable solution for antibody production.
- Potential to impact therapeutics, diagnostics, and research.

Innovation

- Data-driven approach leveraging machine learning and AI.
- End-to-end pipeline with a user-friendly interface.
- Integration of computational methods with experimental validation.
- Potential to advance antibody engineering and design.