Binder MVP Spec. Doc

Build an end-to-end pipeline that ingests any user-provided target structure (small molecule or protein epitope) and outputs codon-optimized DNA sequences for candidate binders, complete with structural and affinity metrics.

Project Goal:

Build a pipeline that, given any target structure (small molecule or protein), automatically:

1. Detects a binding pocket.

2. Generates ≥50 backbone scaffolds.

3. Designs ≥5000 sequences via ProteinMPNN.

4. Validates folding/complex with AlphaFold2 (pLDDT ≥80, RMSD ≤2 Å).

5. Scores ΔΔG ≤–5 kcal/mol in Rosetta.

6. Outputs the top 10 codon-optimized DNA sequences in an Excel file.