

Docking study protocol template

Write this before the first result. Every later choice has then already been made once, calmly.

Study title		Date	
Investigator		Supervisor	

Section	Your entry
1 Question, written so that it could come back negative	
2 Data sources, identifiers, inclusion and exclusion rules, fetch date	
3 Preparation and measurement method with its constants	
4 Validation step and the success criterion, set in advance	
5 Analysis plan, primary and secondary, with sensitivity analyses	
6 What will be reported whatever the result	
7 Limits to be stated	
8 Laboratory or collaborator who could test the prediction	
9 Outputs, notebook, dataset, figures and where they will be deposited	

Feasibility check

- Does the target have several public structures and compounds with public chemistry.
- Can the whole analysis run with free tools on a normal laptop.
- Is the first study small enough to finish, one target family, one comparison, one validation.
- Has the collaborator who would test the prediction been named before the work starts.

Based on the ERAS Africa Molecular Docking using Python course, 2026, and the study "Target Protein Pocket Volume and Antiretroviral Drug Physicochemical Properties" (Hailekiros, 2026) with its reproduction guide. Tool documentation from RDKit, AutoDock Vina, Meeko, RCSB PDB, PubChem and ProteinsPlus. Free to copy and adapt with attribution.