Step	Task Description	Estimated (days)
1.	Select PDB ID: LmrR_pAF (6I8N) Add substrates (enal and indole) Run Qprep Generate the (qmap) for the WT enzyme make FEP file	3
2.	Select all 12 active site residues mentioned in the paper Automate Workflow • Qprep • Minimization • FEP	2
3.	Run EVB alanine scanning simulations on the concerted Friedel–Crafts alkylation reaction for WT and all mutants. • The concerted single-step EVB approach captures the simultaneous formation of the iminium ion with enal and the C–C bond formation to indole	3
4.	Analyze computational results: structure (hydrogen bonds), energy profiles, electrostatics; write draft report.	3
5.	Use enzyme constructs from Roelfes Lab (assuming they are available as per the article).	— (concurrent/assumed available)
6.	Perform enzyme kinetics activity assays on WT and 12 variants • measure initial rates • calculate Km and kcat via Michaelis-Menten kinetics.	7
7.	Analyze product yield via HPLC for all enzyme variants • collect aliquots • quench reactions, prepare samples • run HPLC using internal standards, • quantify products.	7
8.	Writing final report	3