# Target IA and structural analysis protocol contribution to *in silico* drug design

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We developed a protocol by combining the protein structural flexibility with machine learning analysis to improve binding site characterization. Pockets estimation, tracking, druggability prediction and statistical analysis are performed on large samples of simulated conformations obtained by molecular dynamics simulations. Simulation can be performed on unbound or bound RBD forms but also with mutations. Analysis of clusters of pockets allows the characterization of main druggable sites taking into account their flexibility, extraction of key residues and evaluation of the impact of mutations on binding site stability and druggability. Then drug prediction to prevent protein-protein interaction or block the target function can be improved by applying IA and docking approaches on binding site key residue.

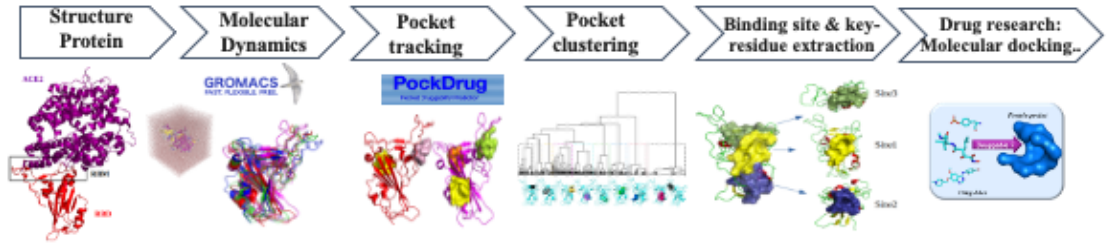


Figure 1: Proposed protocol for improving binding site characterization

Bibliography :

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