

**What is desirable about the structural properties
of a SBDD target?**

- Small
 - less ambiguity regarding binding site
 - more amenable to molecular simulation

- Rigid
 - molecular docking is more accurate
 - molecular simulation requires less sampling

- Binding site is
 - unique, favoring specificity
 - evolutionarily conserved, less susceptible to resistance



What is desirable about the structural properties of a SBDD target?

- Small
 - less ambiguity regarding binding site
 - more amenable to molecular simulation
- Rigid
 - molecular docking is more accurate
 - molecular simulation requires less sampling
- Binding site is
 - unique, favoring specificity
 - evolutionarily conserved, less susceptible to resistance

There are multiple online databases to help you identify suitable targets

- The Special Programme for Research and Training in Tropical Diseases (TDR) Targets (<https://tdrtargets.org/>) - A database that allows you to apply various filters to identify drug targets. Focuses on neglected tropical diseases
- Pocketome (<http://ablab.ucsd.edu/POCKETOME/>) - An encyclopedia of conformational ensembles of druggable binding sites that can be identified experimentally from co-crystal structures in the Protein Data Bank. It can help you investigate whether a structural motif has is druggable and whether it is unique.
- Therapeutic target database (<http://idrblab.net/ttd/>) - “A database to provide information about the known and explored therapeutic protein and nucleic acid targets, the targeted disease, pathway information and the corresponding drugs directed at each of these targets.” This can help you determine precedence for a target.
- BindingDB (<http://www.bindingdb.org/bind/index.jsp>) - “BindingDB is a public, web-accessible database of measured binding affinities, focusing chiefly on the interactions of protein considered to be drug-targets with small, drug-like molecules.” BindingDB can help you determine whether a any small molecule (not necessarily a drug) has been found that binds to a target.