

**experimental
tractability
criteria**

- Multiple protein crystal structures
- Known bacterial expression
- Availability of multiple purchasable known ligands
- Tractable experimental affinity measurements

**isolated
challenge
filters**

- Ligand protonation state and tautomer effects
- Protein protonation state effects
- Protein conformational change upon binding
- Presence of PTMs affecting affinity
- Coordinated metals
- Ordered waters