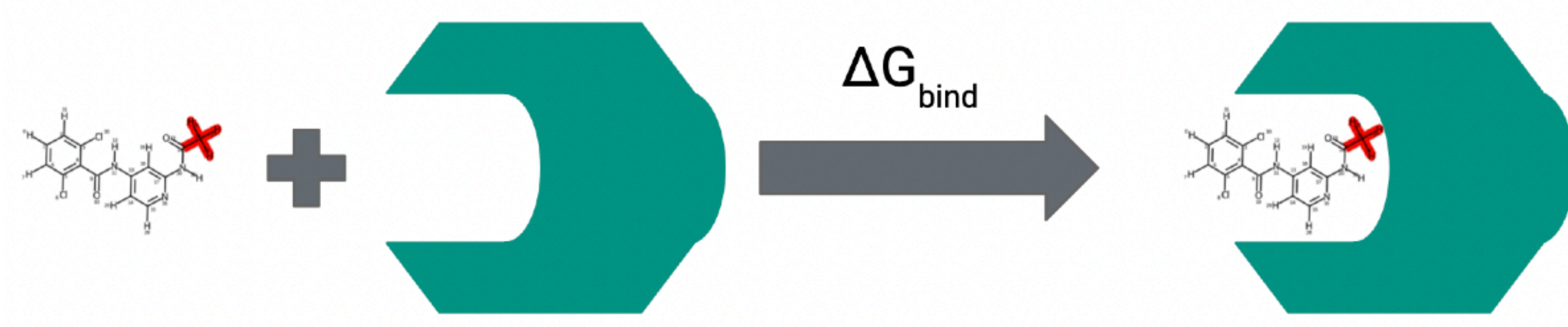


Outline

- Intro: Campaign-scale software
- Path sampling and OpenPathSampling
- **Alchemical free energy transformations and Open Free Energy**
- Best practices to interface with campaign-scale software

Drug design



- Most drugs are only therapeutically active when bound.
- ΔG tells us the relative probability of being bound vs. unbound.
- This makes ΔG an important metric for drug design.