

Discussion questions for
Structure-Based Strategies for Drug Design and Discovery
Kuntz

KHORANA

- Advances that made possible structure-based drug design
- Different aspects of drug design: lead discovery, optimization
- Types of inhibitors (transition-state analog, peptides, etc.)
- Alternate approaches to docking (QSAR, MD, etc.)

CURIE

- Basic idea of how DOCK and similar programs work
- Sampling and scoring, limitations thereof
- Computer power, then and now

ANFINSEN

- Comparing docking predictions to experiment
- Why is computer-aided drug design difficult
- “Can we design drugs from first principles”?