

# Reference-based Docking

Molecule  
Designs

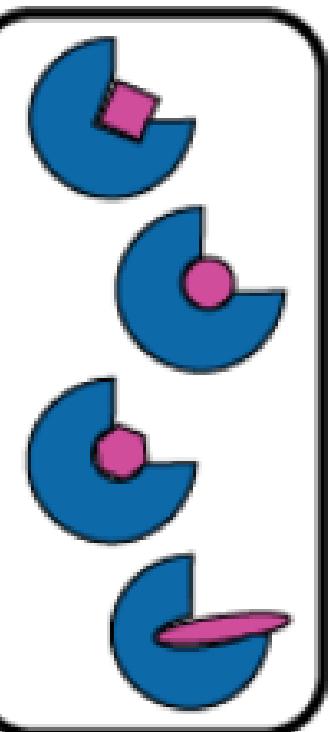


Query  
Ligands

Reference  
Structures



Predicted  
Poses



Ranked Molecules

| Chemist Rank | Docking Score | POSIT Score | FEP pIC50 |
|--------------|---------------|-------------|-----------|
| 3            | -11.01        | 0.85        | 6.8       |
| 1            | -9.79         | 0.97        | 7.1       |
| 2            | -9.83         | 0.54        | 5.2       |
| 4            | -8.99         | 0.64        | 4.49      |
| .            | .             | .           | .         |
| .            | .             | .           | .         |
| .            | .             | .           | .         |