

Reference-based Docking

Molecule
Designs



Query
Ligands

+

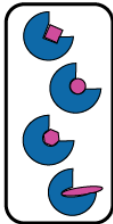
Reference
Structures



Reference
Ligands



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
.	.	.	.
.	.	.	.
.	.	.	.