Molecular Docking: Binding Affinity vs Molecular Weight Bubble size represents binding strength magnitude **Alkannin** -9 kcal/mol **Shikonin** 8.7 kcal/mol Celecoxib -8.2 kcal/mol

9.5

9.0

Binding Affinity (|kcal/mol|)

8.0

7.5

250

Compound Type • Natural Product • Synthetic Drug

Molecular Weight (Da)

350

400

300

Larger bubbles indicate stronger binding affinity