

PubChem Compound
Database
~ 33 million molecules

Filter based on 80% Tanimoto
similarity coefficient then using
Lipinski's rule of five

Epothilone A Paclitaxel Discodermolide Laulimalide Eleutherobin Sarcodictyin A

Merge all filtered
compounds

1591 Molecules

Delete all duplicates

737 Molecules

Clustering and diversity subset
based on 90% Tanimoto
coefficient

645 Molecules

Docking and scoring

First 25 hits

