

A**WT**

Pocket F

Pocket A

Pocket E

Pocket B

Pocket C

B**G177D mutant**

Pocket F

D177

C

1) SBVS

500,000 Enamine diversity library

2) LBVS (substructure search)/SBVS

7,000,000 MolPort library

WT pocket B**G177D pocket F**

1) 500,000 Enamine diversity set

2) 240,000 LBVS hits

2) 48 LBVS hits

SBVS

Hit triage

1) 2,000 hits

2) 2,000 hits

1) 2,000 hits

2) 48 hits

Hit triage (cont.):

- Diversity analysis
- Re-scoring

1) 11 hits

2) 37 hits

1) 46 hits

2) 8 hits

10 experimentally validated hits (SPR)