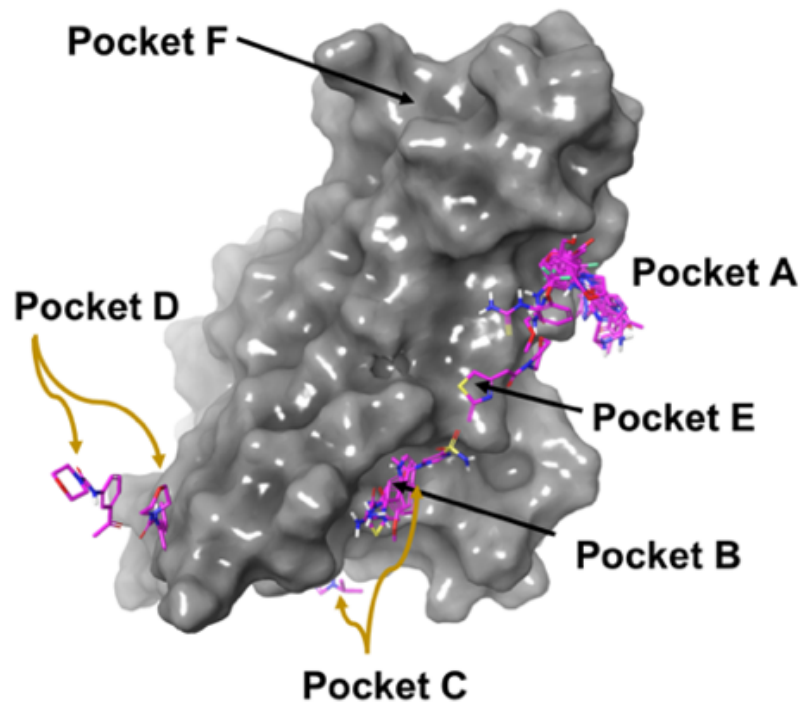
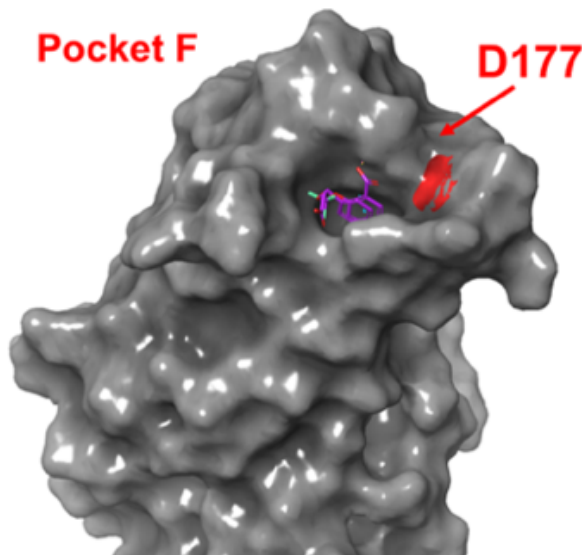


A**WT****B****G177D mutant****C**

- 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	1) 500,000 Enamine diversity set
2) 240,000 LBVS hits	2) 48 LBVS hits

- | | |
|----------------------------------|----------------------------------|
| 1) 500,000 Enamine diversity set | 1) 500,000 Enamine diversity set |
| 2) 240,000 LBVS hits | 2) 48 LBVS hits |

SBVS
Hit triage

- | | |
|---------------|---------------|
| 1) 2,000 hits | 1) 2,000 hits |
| 2) 2,000 hits | 2) 48 hits |

Hit triage (cont.):

- Diversity analysis
- Re-scoring

- | | |
|------------|------------|
| 1) 11 hits | 1) 46 hits |
| 2) 37 hits | 2) 8 hits |

10 experimentally validated hits (SPR)