

Drugs are designed to optimize interactions

- There is a combinatorial explosion of ways to modify a small organic molecule to make it bind better

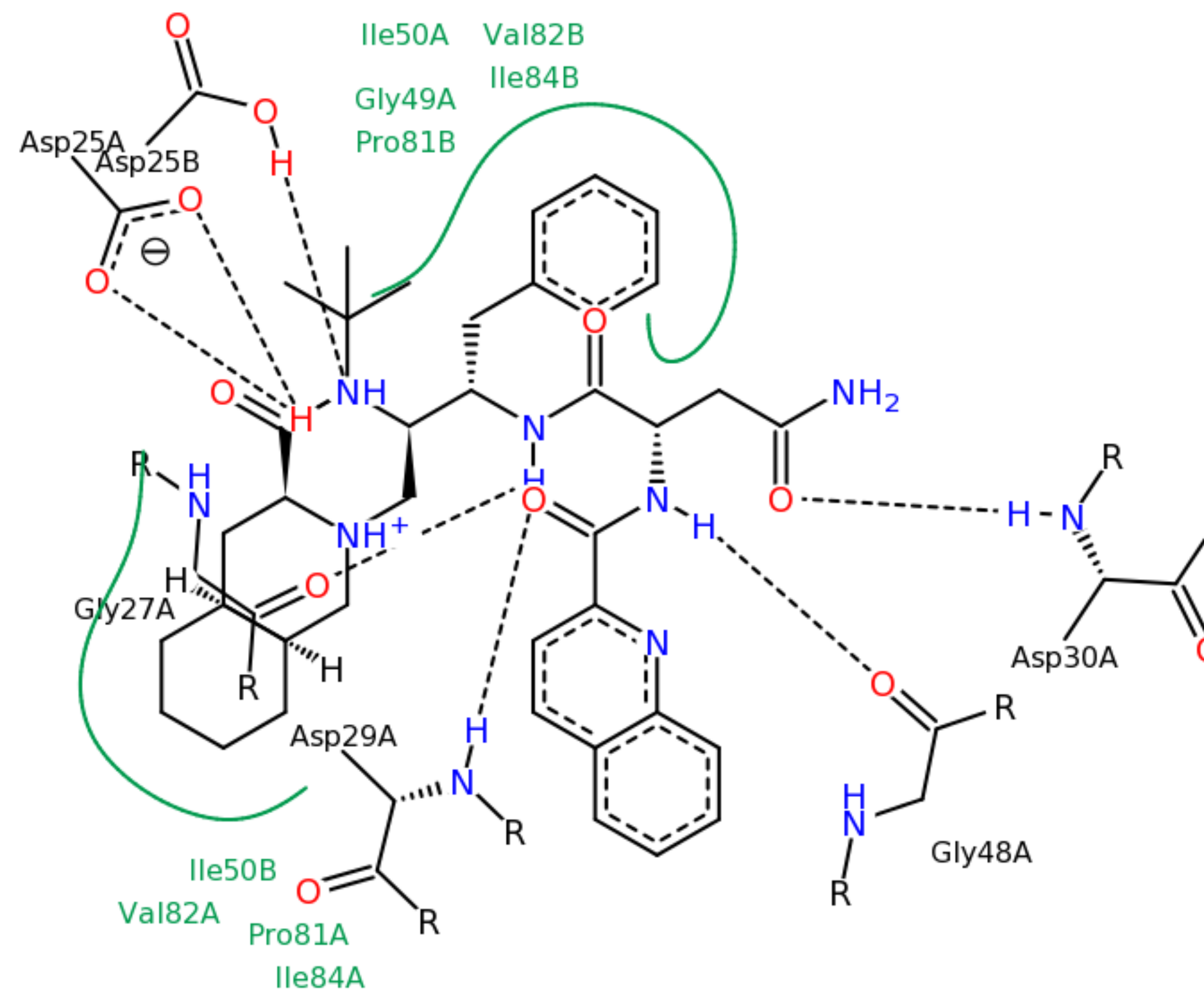
- Structure-based drug design (SBDD) uses the target's structure to
 - maximize interactions that favor binding
 - minimize interactions that disfavor binding



http://www.rcsb.org/pdb/101/motm_disused_entry.do?id=1hxb

Drugs can be designed to optimize interactions

- There is a combinatorial explosion of ways to modify a small organic molecule to make it bind better
- Structure-based drug design (SBDD) uses the target's structure to
 - maximize interactions that favor binding
 - minimize interactions that disfavor binding



http://www.rcsb.org/pdb/101/motm_discussed_entry.do?id=1hxb

Interactive Structural Visualization Exercise