What is molecular docking good for?

- Predicted structure can
  - explain behavior, e.g. mutagenesis
  - facilitate molecular design, e.g. of pharmaceuticals
- Predicted scores can be used for virtual screening

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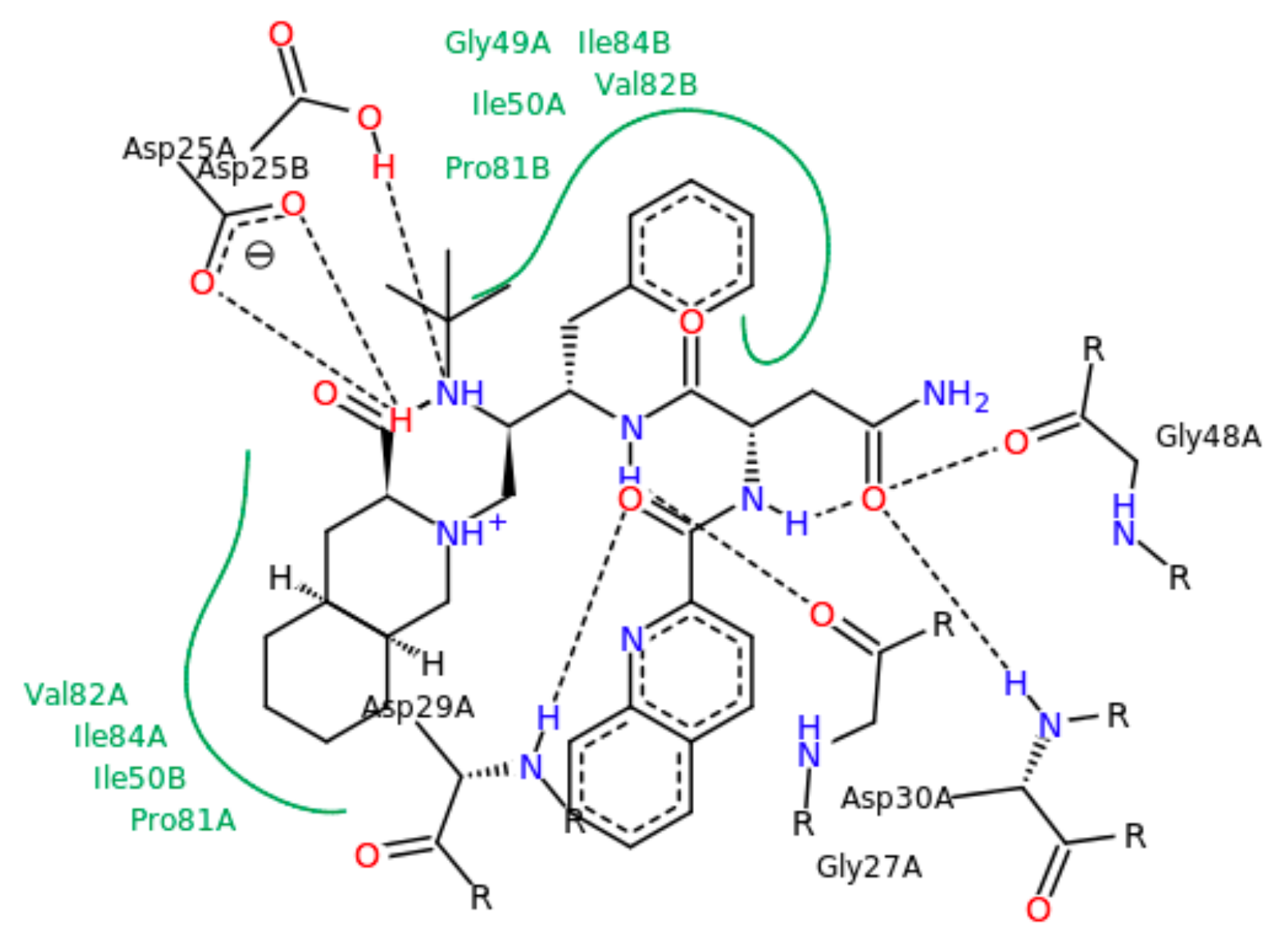
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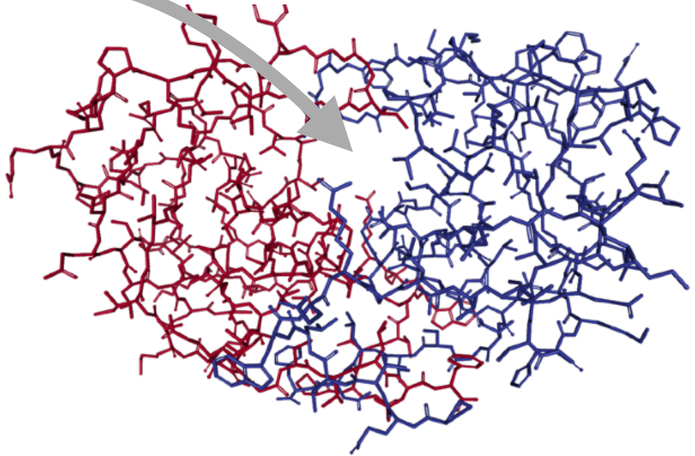

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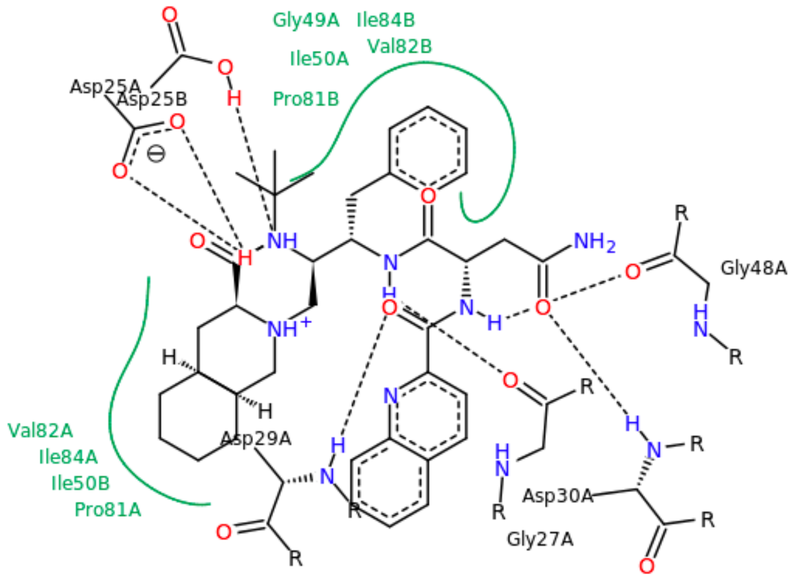

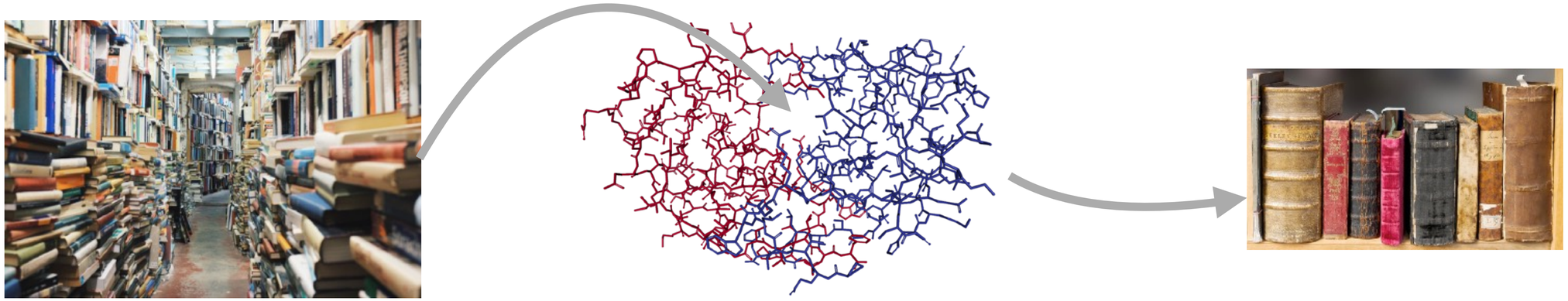

How does docking work?

- Docking is optimization of a scoring function, E(x)
  - E can be the total potential energy or interaction energy
    - can be entirely physics-based or partly knowledge-based
    - physics-based are usually molecular mechanics energies
  - x is a vector describing the molecular coordinates
- Optimization algorithms include
  - anchor-and-grow in UCSF DOCK, the original docking program
  - genetic algorithm in AutoDock, the most popular docking program
  - Fast fourier transform, especially for fragment and protein-protein docking