General information about Molecular docking

- **molecular docking** → links protein structure and conserved motifs to ligand binding through efficient computational optimization, generating testable hypotheses for biological and pharmaceutical research.

- Molecular docking is a computational method that predicts how a ligand binds to a protein in 3D space and estimates binding affinity.
- Docking involves pose sampling and energy scoring, not time-based simulation.
- Docking results are predictive, not experimental proof.
- Protein motifs are short conserved sequence or structural patterns that define functional or binding regions.
- Docking does not identify motifs but tests how ligands interact with motif residues.
- Strong docking poses often involve conserved motif amino acids, explaining motif conservation.
- Docking is used to validate motif function, guide drug design, and interpret resistance mutations.
- It helps study enzyme–substrate, drug–target, and peptide–protein interactions.
- Spa typing and sequence alignment are not docking-related, but docking may use limited alignment only for structure preparation, not typing.
- High-resolution mass spectrometry (HRMS) provides exact mass confirmation, often used alongside docking in research for compound validation.
- Lamarckian Genetic Algorithms (LGA) combine genetic algorithms with local search, allowing inherited improvements.
- LGA is widely used in docking to balance global exploration and local refinement of binding poses.
- Docking is often followed by molecular dynamics simulations and wet-lab assays to confirm predictions.
- **AutoDock Tools** functions as a **pre- and post-processing interface** for molecular docking.