How is a chemical library prepared for virtual screening?

- Chemicals in libraries are usually specified by a string of characters
  - Simplified Molecular-Input Line-Entry system (SMILES)
    - Element abbreviation, possibly in square brackets
    - Bonds between atoms
  - IUPAC International Chemical Identifier (InChI)

- Docking requires 3D structures and molecular mechanics parameters
  - Conformer generation programs such as OpenEye Omega or Balloon can be used to create 3D structures. ZINC provides 3D structures based on Omega.
  - In AutoDock, parameters for each ligand atom are the partial charge and atom type

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What is a virtual screening hit and what are some desirable properties of a hit?