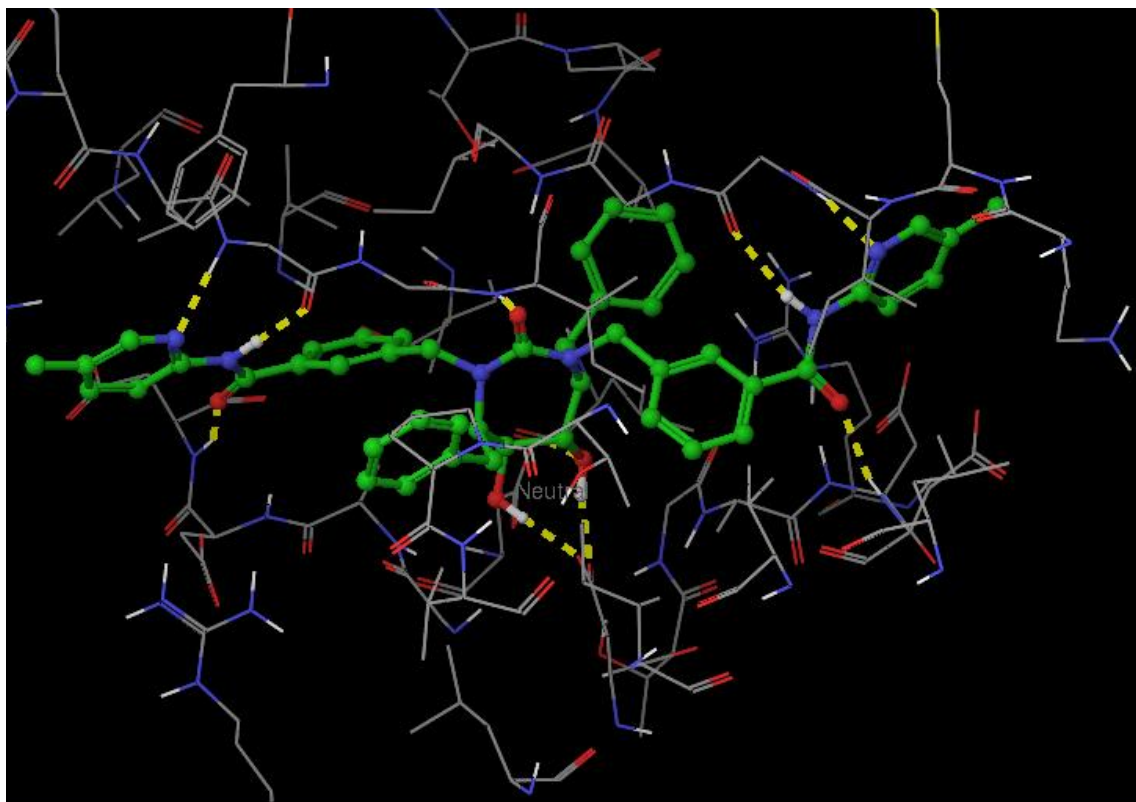


Ligand Based Virtual Screening



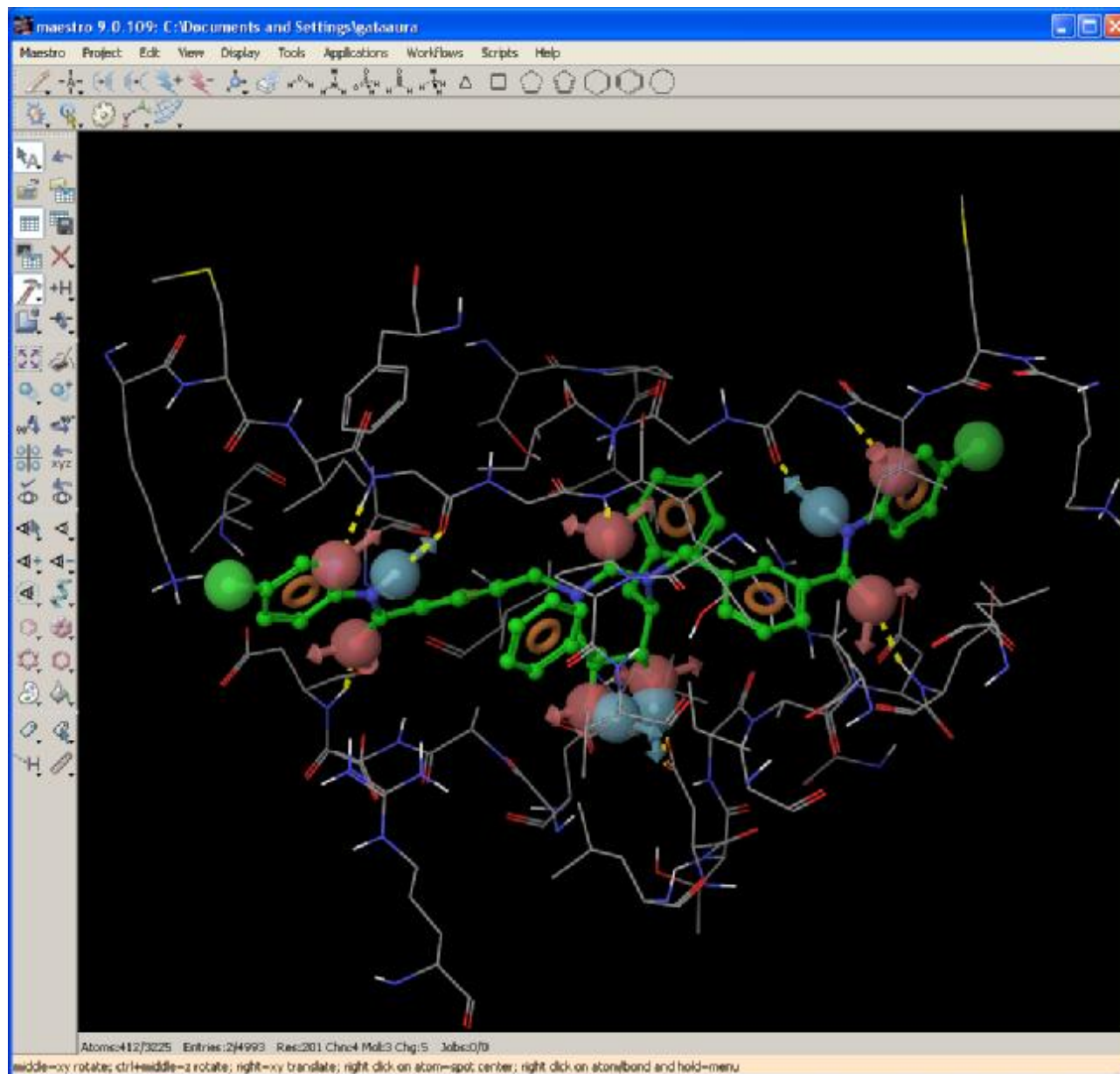
SCHRÖDINGER.

Basic Concepts of Pharmacophores



**The Protein
Shows The
Precise
Nature Of
The
Interactions**

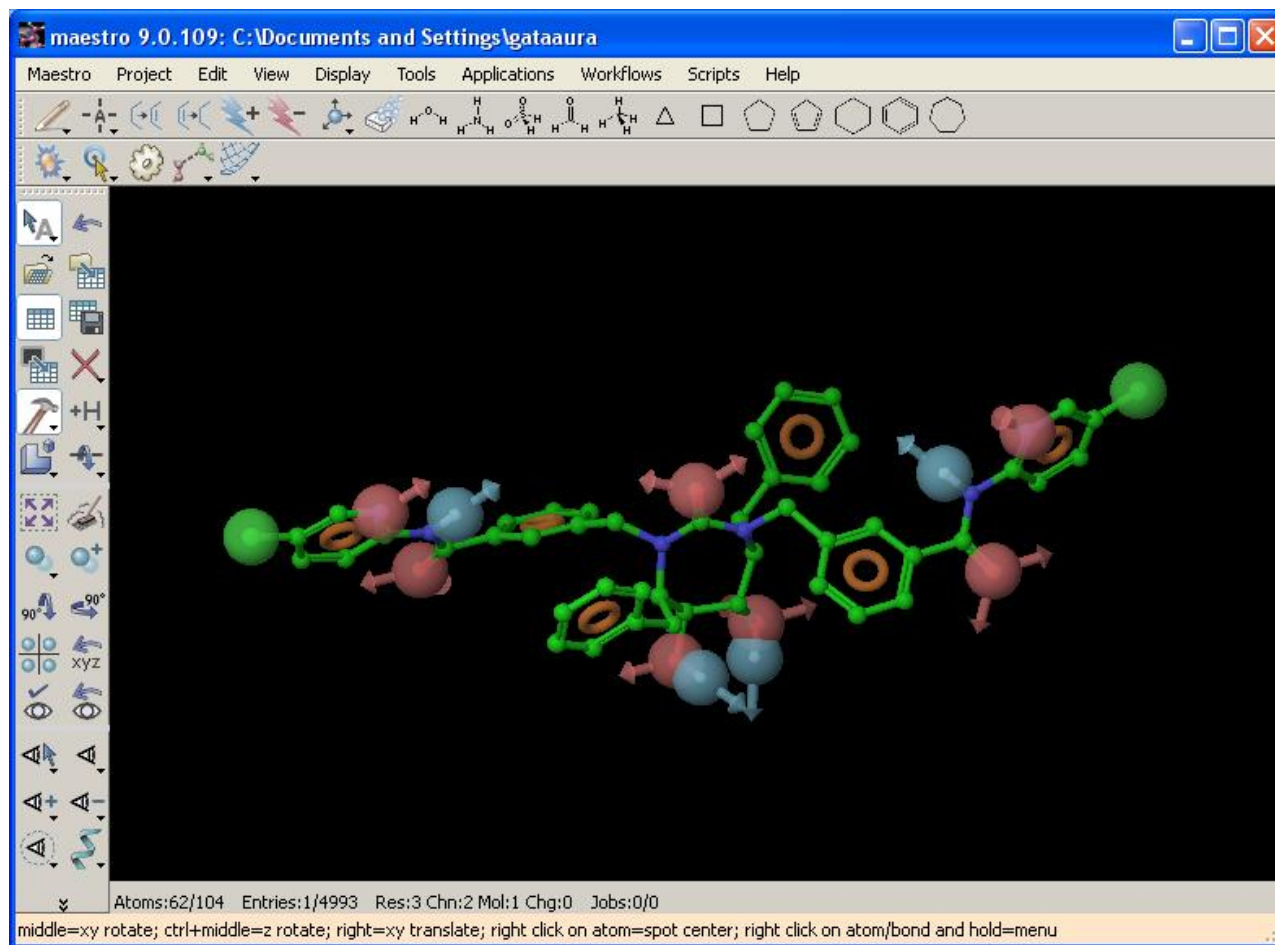
Basic Concepts of Pharmacophores



**Translate
these
Interactions
into ligand
features
A D N P R H**

SCHRÖDINGER

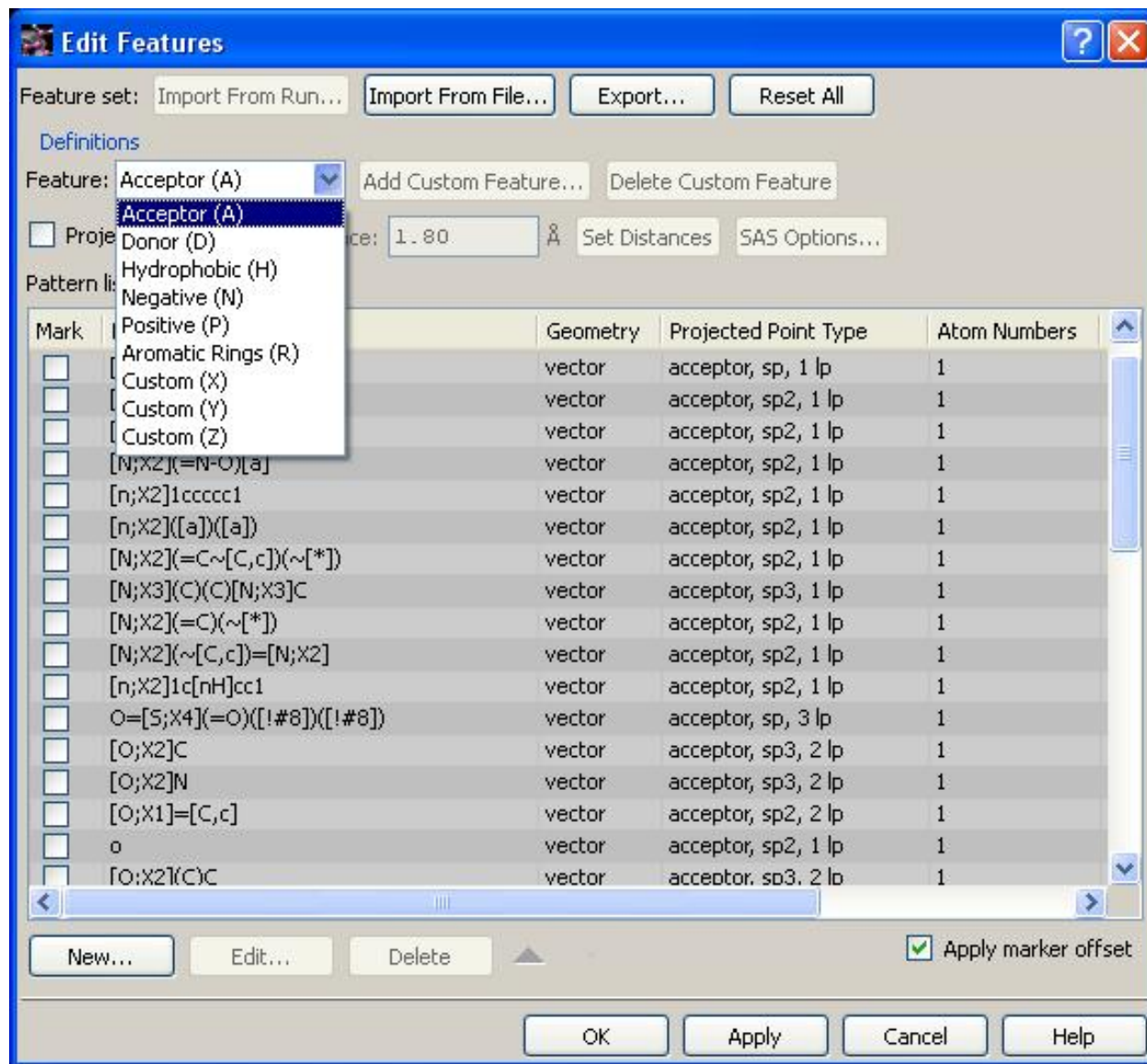
Starting Point for Pharmacophore Development



**The Structure Of
The Ligands Alone
Determine These
interactions...Meas
ure of similiarity to
understand what
infers experimental
activity**

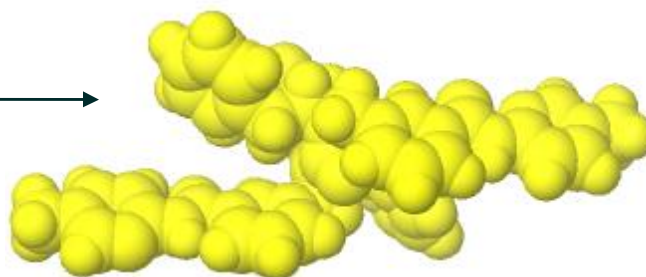
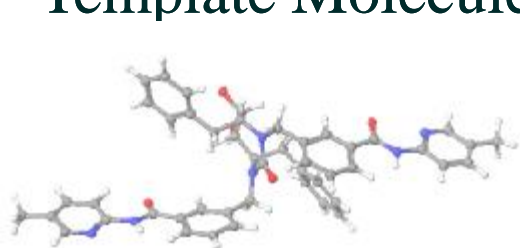
**All done in
absence of protein!**

Features are defined by SMARTS patterns in Phase



Options for Reference Shape

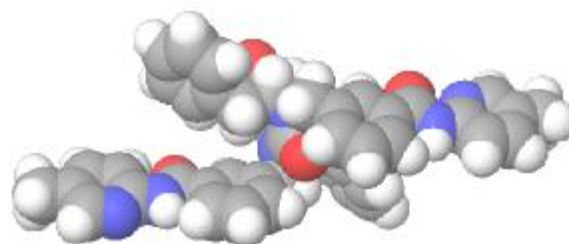
Template Molecule



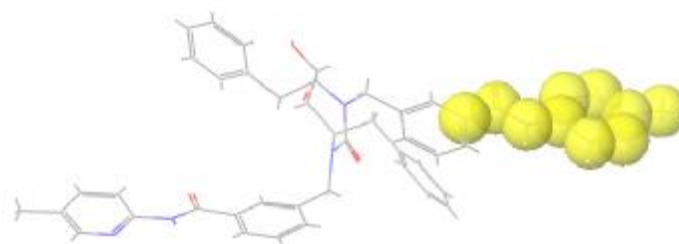
Hydrogens ignored
by default

Atom Typing Schemes

- None
- MacroModel
- Elemental
- Phase QSAR



- Included Volumes
- Excluded volumes (Rec/ Inactives)
- Custom weights
- DB or on-the-fly conformations



SCHRODINGER

Maestro Shape Alignment

