Ligand building with ARP/wARP

Hands-on Tutorial

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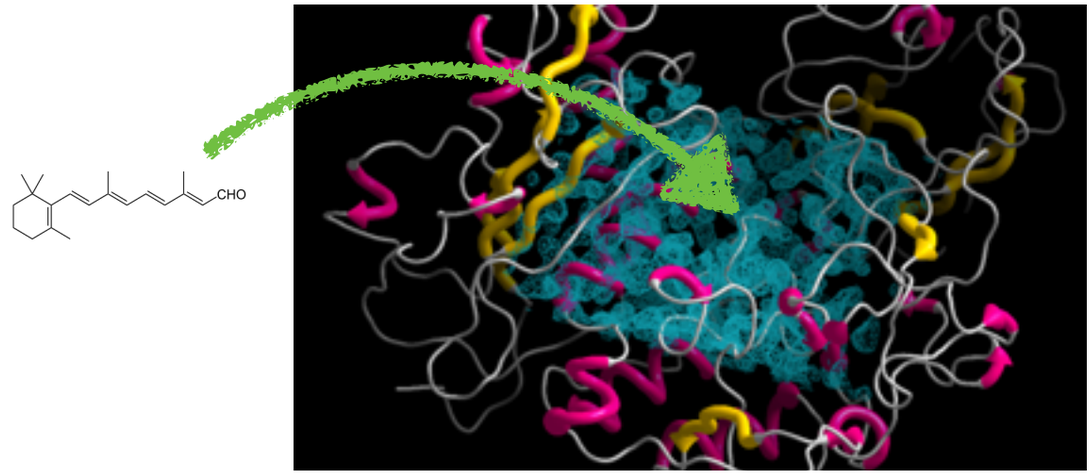
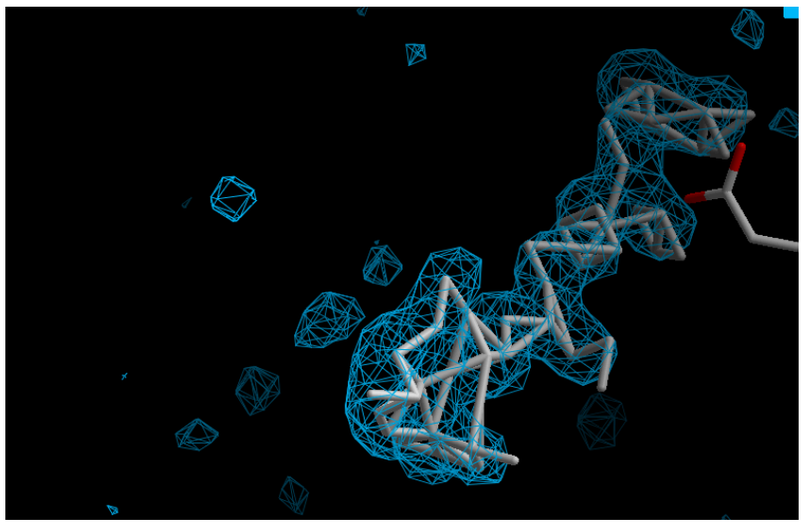
What will you learn?

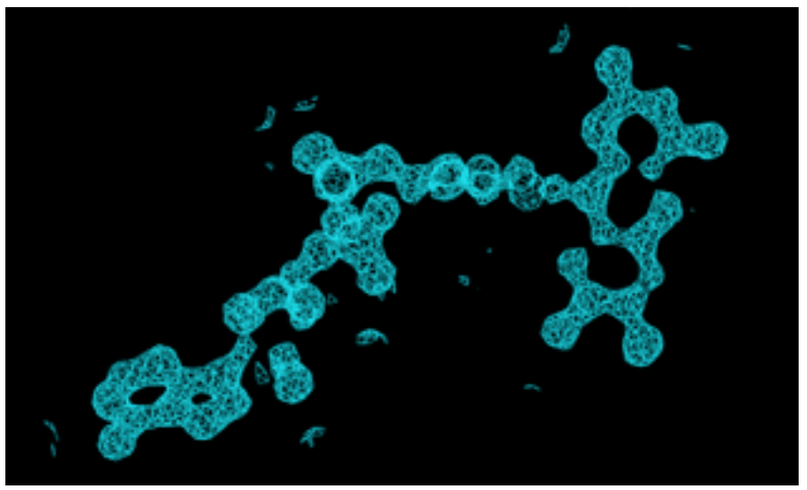
1. Fit a ligand into the electron density



2. Identify a ligand binding site on the electron density



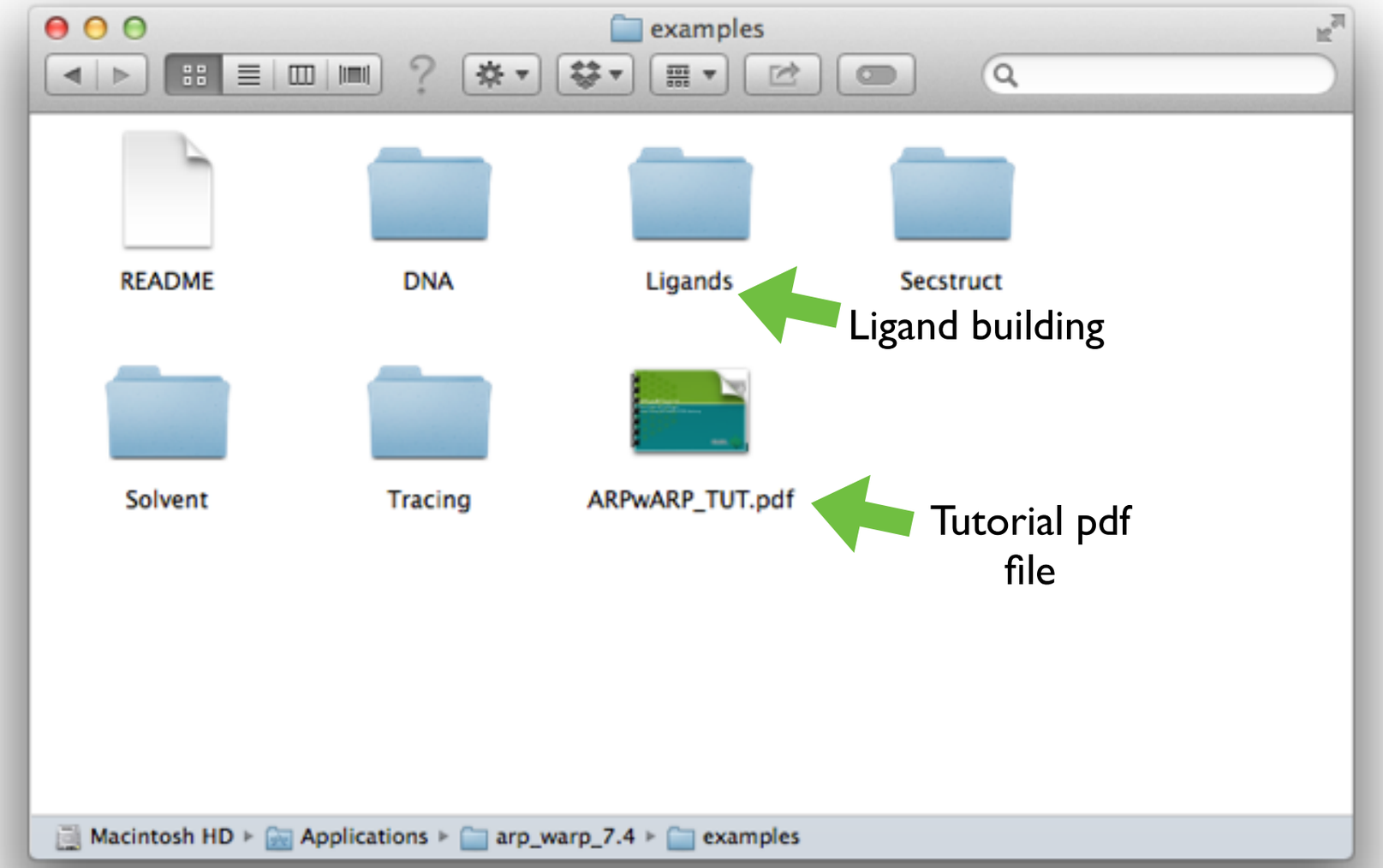
3. Identify a ligand on the electron density



What do you need?

Example data:

Applications → arp/warp_7.4 → examples



What do you need?

- MTZ file (e.g, 1cbs.mtz)
- Difference map (e.g., 1CBS_noligand_diff.map)

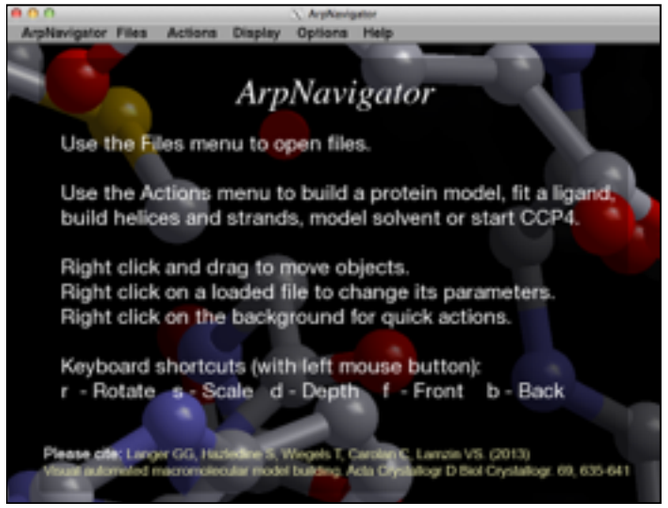
One of these

- APO structure (e.g., 1CBS_noligand.pdb)
- Ligand template (e.g., RETINOICACID.pdb)

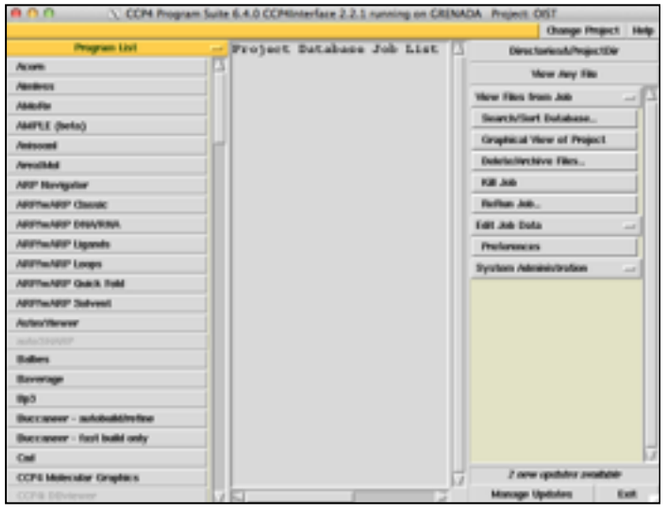
Not for ligand identification

How to start it?

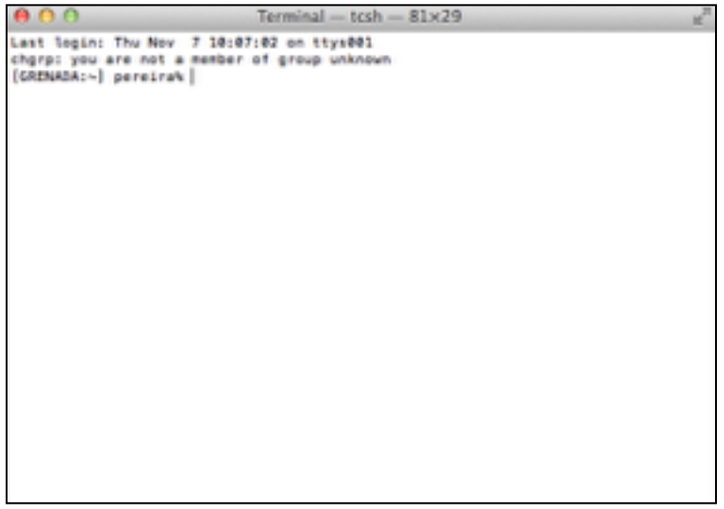
3 ways:



ArpNavigator



CCP4 Suite



Terminal

This tutorial!

```
$warpbin/auto_ligand.sh [parameters]
```

Check the user guide!