Ligand fitting trial 1.

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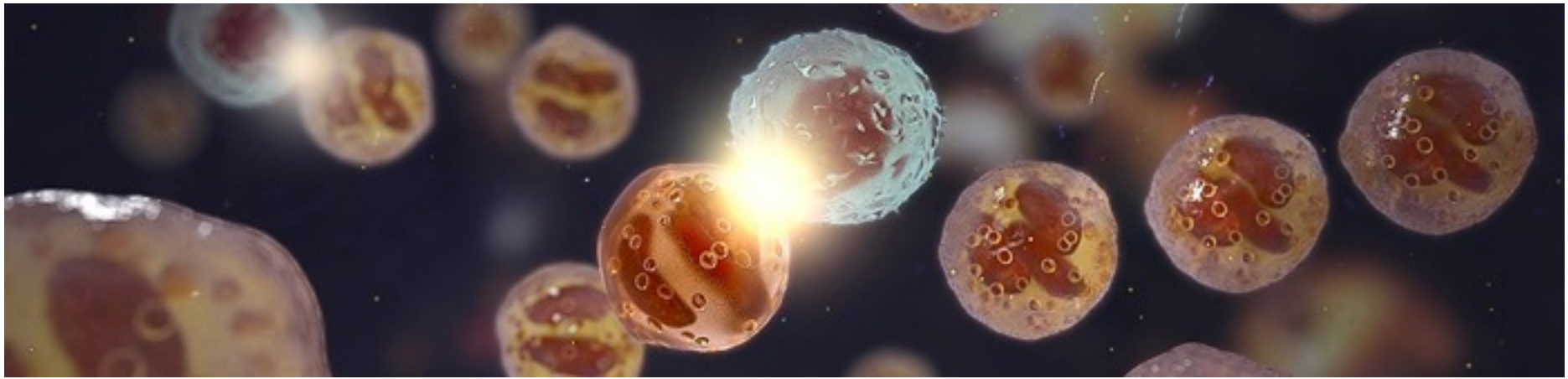
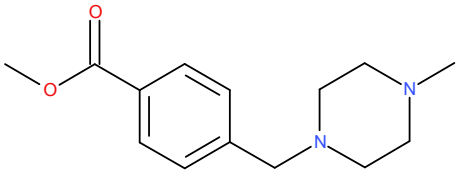
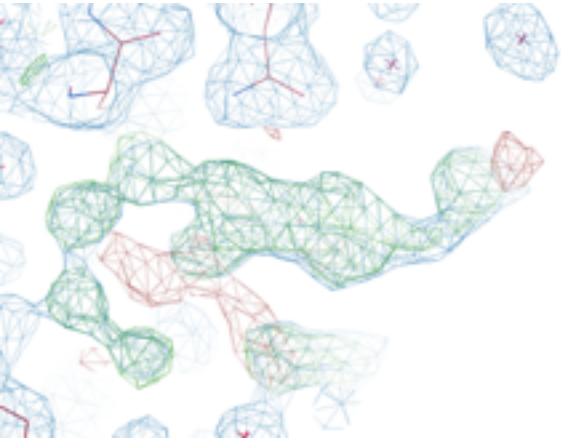
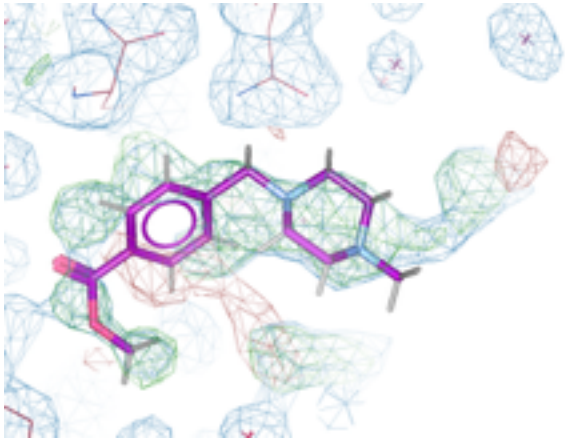


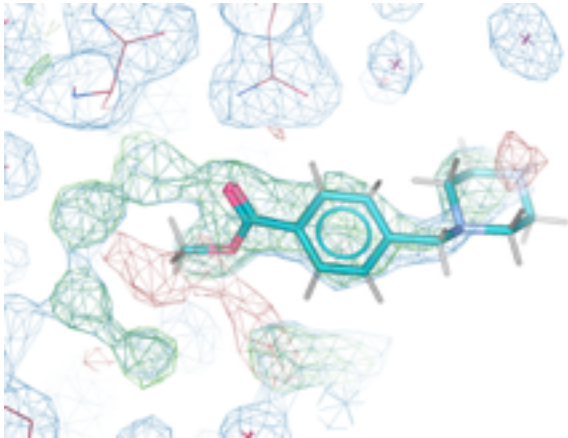
Problem 1.



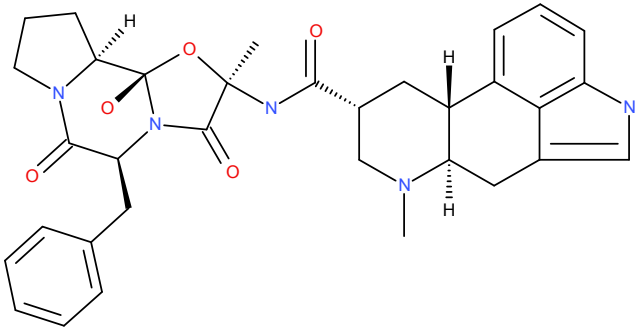
- straight forward ligand fitting workflow
- smi → pdb, cif with grade, acedrg and pyrogen
  - acedrg fell over on the smi file if it contained description string and made piperazine ring boat (version issue?)
- basic ligand fitting in coot
  - coot misplaced the ligand – due to unmodelled water positions?
  - ligand expert should be default
- manual intervention: fix pose
- piperazine ring probably disordered



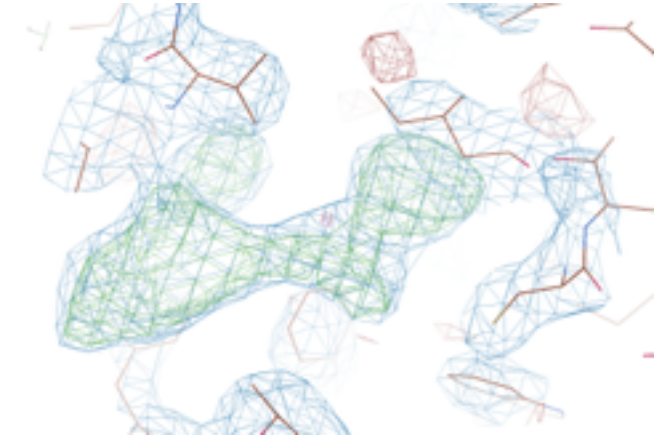


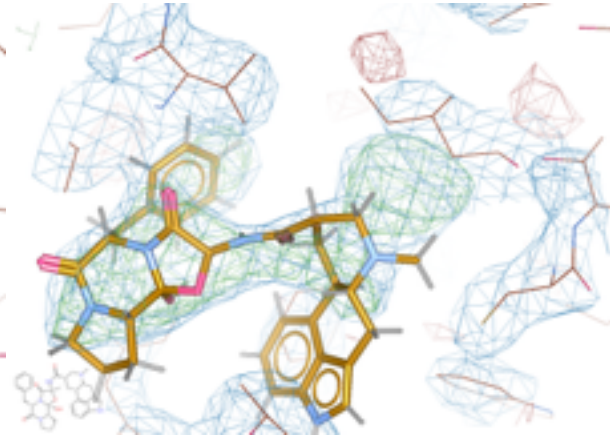


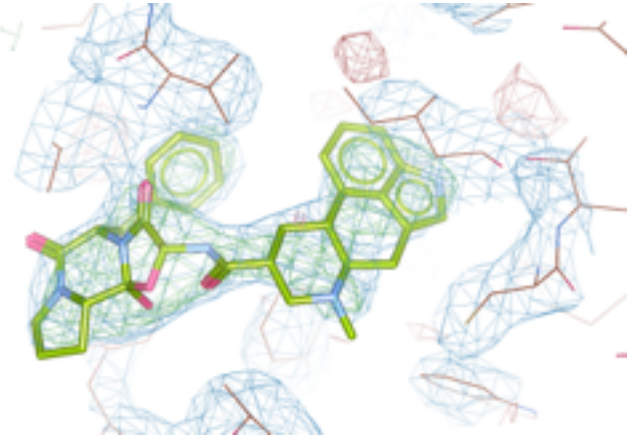
Problem 2.



- moderate resolution GPCR and triptamine ligand workflow
- smi → pdb, cif – see previous slide, all three OK
- basic ligand fitting in coot – see previous slide
- manual intervention: fix pose
- examine interactions…
- It seems essential to have the right (latest?) versions of all CCP4 tools installed to work well together. My current coot installation can't reach pyrogen, not clear how to link it to acedrg.
- i2 still too slow on a remote NFS setting to be usable.



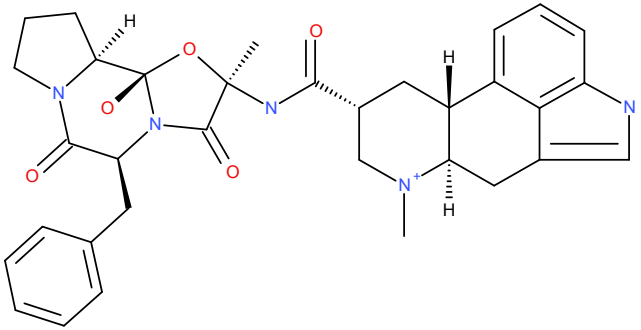


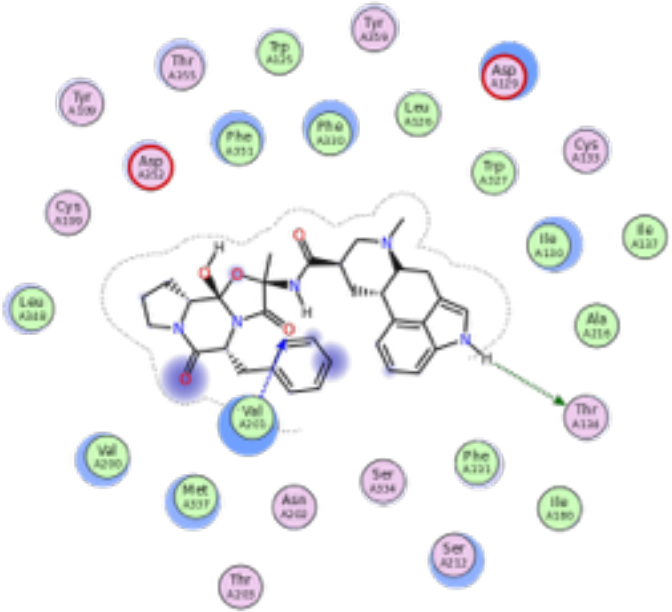


Problem 2.

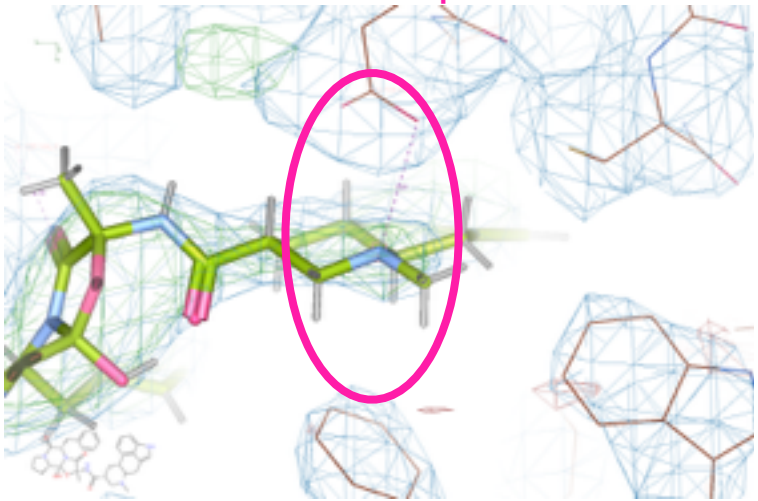
- examine interactions… → fix protonation
  Why do we have to fix it manually?
- ligand modification: use terminal Phe to grow

Flev does not know about salt bridges.





salt bridge missing
N should be protonated



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