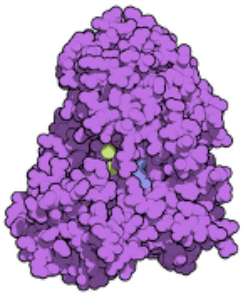

LightDock

FAQ: Frequently Asked Questions

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1. General

1.1. What is *ab initio*?

Blinded docking or *ab initio* is the protocol to execute when no additional information is provided for performing the docking (residue restraints, etc.).

Default recommended protocol is:

- **Swarms**: 400
- **Glowworms**: 300
- **Steps**: 100

In the original publication the number of steps was equal to 200, but quality of the results is not affected using 100 steps. The reason behind performing 200 steps was for benchmarking the method.

2. Setup

2.1. Removing previous files when setup fails

If LightDock setup fails and no `setup.json` file is generated, all files generated by LightDock should be deleted. This is critical as LightDock may append PDB structures parsed to `lightdock_*.pdb` existing

PDB files, with the result of multiple structures per PDB file.

3. Simulation

3.1. DFIRE fails with KeyError

DFIRE scoring function fails with a similar error to this example:

```
File "/home/software/lightdock/lightdock/scoring/dfire/driver.py", line 152, in _g
et_docking_model
anuma = atomnumber[rec_atom_type]
KeyError: 'LYSH1'
```

This is caused by DFIRE scoring functions not recognizing `H` (hydrogen) atoms. Remove all hydrogen atoms and any other non-standard residue or `HETATM`.

For removing hydrogens, you can use the flag `--noh` in `lightdock_setup` command or the Reduce software:

```
reduce -Trim input.pdb > output.pdb
```