
modeller_script Documentation

Release 1.0.0

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Contents:

1. QUICK START

1.1. REQUIREMENTS

- On IENA :

module add modeller/9.11

- Otherwise add the following expression in your bashrc :

```
export PYTHONPATH=/usr/lib/modeller9.11/modlib:/usr/lib/modeller9.11/lib/x86_64-  
intel8/python2.5:$PYTHONPATH export LD_LIBRARY_PATH=/usr/lib/modeller9.11/lib/x86_64-  
intel8:$LD_LIBRARY_PATH
```

And : source .bashrc

1.2. RUN

To get the description of script options :

`modeller_script.py -h`

- First case: one alignment (template + model) + pdb (template)

`modeller_script.py -i alignment.pir -p structure.pdb`

- Second case: one multifasta (template + model) + pdb (template) + alignment with clustalo

`modeller_script.py -f sequences.fasta -p structure.pdb -a clustalo -g path/to/clustalo/`

- Third case: modelize with several template and set 3 hetero atom from only one of these structures:

`modeller_script.py -f sequences.fasta -p structure1.pdb structure2.pdb -ht 3 -hm Model_name Structure1_name`

INDICES AND TABLES

- *genindex*
- *modindex*
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