Structure threader

Opis

Program za paraleliziranje i automatiziranje pokretanja softvera **Structure**, **fastStructure**, **MavericK** i **ALStructure**.

Dostupne verzije

Verzija	Modul	Supek	Padobran
1.0	scientific/structure_threader/1.0	✗	✓

Primjer korištenja

- structure_threader je dopremljen sa apptainerom tako da se mora koristiti **structure_threader.sh** wraper
- za flag -st potrebno je dati putanju za željeni structure
  - str_bin=/usr/local/bin/structure
  - str_bin=/usr/local/bin/fastStructure
  - str_bin=/usr/local/bin/MavericK

st.pbs

```
#!/bin/bash

#PBS -N structure_threader-ex
#PBS -l select=1:ncpus=64:mem=16GB
#PBS -j oe
#PBS -q cpu

cd $PBS_O_WORKDIR

module load scientific/structure_threader/1.0

str_bin=/usr/local/bin/structure

structure_threader.sh structure_threader run -i scilla_m10/scillastructureisabella_EDITED.txt -K 8 -R 10 --
params scilla_m10/scillastructureisabella_mainparams.txt -o scilla_m10/results_edited_10 -t $NCPUS -st
${str_bin}
```