

DIAMOND

Dostupne verzije i pripadajući moduli:

Verzija	Modul
2.1.6	bioinfo/DIAMOND/2.1.6
2.1.7	bioinfo/DIAMOND/2.1.7

Korištenje:

Primjer je skinut s : <https://scop.berkeley.edu/downloads/scopeseq-2.07/astral-scopedom-seqres-gd-sel-gs-bib-40-2.07.fa>

Radeno po tutorialu: <https://github.com/bbuchfink/diamond/wiki/1.-Tutorial>

makedb.sge

```
#!/bin/sh
#$ -N makedb
#$ -pe *mpisingle 8
#$ -cwd

module load bioinfo/DIAMOND/2.1.6

diamond makedb --in astral-scopedom-seqres-gd-sel-gs-bib-40-2.07.fa -d astral40 --threads $NSLOTS
```

blastp.sge

```
#!/bin/sh
#$ -N blastp
#$ -pe *mpisingle 8
#$ -cwd

module load bioinfo/DIAMOND/2.1.6

diamond blastp -q astral-scopedom-seqres-gd-sel-gs-bib-40-2.07.fa -d astral40 -o out.tsv --very-sensitive
```

Korištenje clusteringa u diamondu zahtjeva više RAM-a. Stoga je potrebno definirati sa opcijom -M.

Primjer je skinut s : <https://scop.berkeley.edu/downloads/scopeseq-2.07/astral-scopedom-seqres-gd-sel-gs-bib-95-2.07.fa>

Ovdje uzimamo 8 threadova po 5 GB radne memorije: $8 \times 5 = 40$ taj broj proslijedimo opciji -M

cluster.sge

```
#!/bin/sh
#$ -N clustering
#$ -pe *mpisingle 8
#$ -cwd
#$ -l memory=5

module load bioinfo/DIAMOND/2.1.6

diamond cluster -d astral-scopedom-seqres-gd-sel-gs-bib-95-2.07.fa -o clusters.tsv --approx-id 40 -M 40G --header --threads $NSLOTS
```

Instalacija:

mamba

```
source /apps/mambaforge/mamba/bin/activate  
mamba create -p /apps/virtenv/DIAMOND/2.1.6 -c bioconda diamond
```