AlphaFold 2 run on IGBMC HPC

Clément script

```
#!/bin/bash
#SBATCH --mail-type=ALL
#SBATCH --mail-user=charentc@igbmc.fr
#SBATCH --cpus-per-task 2
#SBATCH --gres=gpu:a3g.20gb:1
#SBATCH --mem=50G
#SBATCH -p gpu

module load alphafold/2.3.2
AF=/shared/genomes/alphafold2/2023-04-28

srun run_alphafold.sh \
    --data_dir=$AF/ \
    --output_dir=$(pwd)/ap_out \
    --fasta_paths=Test.fasta \
    --max_template_date=2020-05-14 \
    --db_preset=full_dbs \
    --
bfd_database_path=$AF/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sort
ed_opt \
    --
uniref30_database_path=$AF/uniclust30/uniclust30_2018_08/uniclust30_2018_08
\
    --uniref90_database_path=$AF/uniref90/uniref90.fasta \
    --mgnify_database_path=$AF/mgnify/mgy_clusters_2018_12.fa \
    --template_mmcif_dir=$AF/pdb_mmcif/mmcif_files \
    --obsolete_pdbs_path=$AF/pdb_mmcif/obsolete.dat \
    --use_gpu_relax=True \
    --model_preset=monomer \
    --pdb70_database_path=$AF/pdb70/pdb70
```

From:
https://bsi.inscog.eu/ - **BSI wiki**

Permanent link:
https://bsi.inscog.eu/doku.php?id=alphafold

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