Steps for online MSA generation, afv3

1. Make folder for project. For example, make a folder names online_MSA_afv3
   1. *Mkdir online_MSA_afv3*
2. Upload fasta file to "online_MSA_afv3"
   1. *Vi test_models_afv3.fasta*
3. Upload the python scripts (pipeline_CFB) to current folder
   1. *Scp –r Downloads/ pipeline_colabfold_batch_onlineMSAgen vmischley@login.expanse.sdsc.edu:/expanse/lustre/projects/was136/vmischley/online_MSA_afv3*
4. Run the script: run_pipeline_CFB_onlineMSAgen.py. This will split the fasta file into individual fasta files with sequences that will in total take less than 48 hours to complete. It will then create the submit script. Input needed is path to fasta file (use full file path) , number of recycles and version of AF
   1. *Python pipeline_colabfold_batch_onlineMSAgen/run_pipeline_CFB_onlineMSAgen.py /expanse/lustre/projects/was136/vmischley/online_MSA_afv3/test_models_afv3.fasta 12 alphafold2_multimer_v3*
5. Change into the model folder where all of the submit scripts are
   1. *Cd models*
6. Submit all of the submit scripts
   1. *Sbatch 1_CFB_test_models_MSA_1_submit.slurm*

7. Run move_af.py to copy only pdb files and .json files into one folder (optional). If using move_af.py you must run an interactive node, or else you run out of memory. Input is path to model folder. Output is folder named combined_models
   1. *srun --partition=debug --pty --account=was138 --nodes=1 --ntasks-per-node=4 --mem=32G -t 00:30:00 --wait=0 --export=ALL /bin/bash*
   2. *Python move_af.py /expanse/lustre/projects/was136/vmischley/cluster_MSA_afv2/test_models*

8. After completion, download folder