alphafold3

method one: via alphafold 3 server

- alphafold server only accepts limited number of liginds (by there CCD ID not SMILE format)
- I experienced running a docking job with this input :

input.json

and got this output:

fold_protein_ligand_docking_job.zip

the server is easy yo use and you can format multi jobs in a json format and submit it (computation is better of course) but liginds are limited .

Allowed ligands: `CCD_ADP`, `CCD_ATP`, `CCD_AMP`, `CCD_GTP`, `CCD_GDP`, `CCD_FAD`, `CCD_NAD`, `CCD_NAP`, `CCD_NDP`, `CCD_HEM`, `CCD_HEC`, `CCD_PLM`, `CCD_OLA`, `CCD_MYR`, `CCD_CIT`, `CCD_CLA`, `CCD_CHL`, `CCD_BCL`, `CCD_BCB`

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method 2: using colab

alphafold cannot be imported to colab directly, although there is third-party options, I tried:

colabfold: lightweight implementation of AlphaFold but does not support protein-ligand docking.

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a lighter version that does not requre 1T storage > https://github.com/Kuhlman-Lab/alphafold3?tab=readme-ov-file

I did the **Kuhlman Lab Installation of AlphaFold3 in colab >> check here**

everything went fine until now, I still need to wait for their permission for model weights

```
Successfully built alphafold3
Installing collected packages: alphafold3
Successfully installed alphafold3-3.0.0
```