My code path:

/nfs\_beijing/kubeflow-user/zhangyan\_2023/code/

Conda:

source activate /nfs\_baoding\_ai/zhangyan/xtrimofast

 /nfs\_beijing\_ai/zhangyan\_2023/xtrimofast

/home/zhangyan\_2023/miniconda3/envs/xtrimomultimer

机器：

堡垒机：[堡垒机-堡垒机 (biomap-int.com)](https://relay01.biomap-int.com/#/desktop)

172.30.0.64：22 8099

开通机器初始密码 YjQwOWM4ODAwZjIw

Codeserver:   
/pfs\_beijing/xumeng/code-server-4.4.0-linux-amd64  
cat test.log  
cat start\_vscode.sh

12345678

Docker:

docker pull harbor.biomap-int.com/yiwu/xtrimo:v5.1  
nvidia-docker run -it --privileged --name Zhangyan --shm-size 4G -v /nfs\_baoding\_ai:/nfs\_baoding\_ai -v /nfs\_baoding:/nfs\_baoding -v /pfs\_beijing:/pfs\_beijing -v /nfs\_beijing:/nfs\_beijing harbor.biomap-int.com/zhouyi/docking-benchmark:v1.0

harbor.biomap-int.com/yiwu/xtrimo:v5.1

docker:

 harbor.biomap-int.com/zhouyi/docking-benchmark:v1.0

harbor.biomap-int.com/shaochuan/xtrimo:v3

docker run:

nvidia-docker run -it  --shm-size 64G -v /nfs\_baoding\_ai:/nfs\_baoding\_ai -v /nfs\_baoding:/nfs\_baoding -v /pfs\_beijing:/pfs\_beijing -v  启动docker

code distance:

/nfs\_baoding\_ai/shaochuan/code/ds\_check/epitope\_mp.py

/nfs\_baoding\_ai/shaochuan/code/dock/module1\_docking/src/utils.py

/nfs\_baoding\_ai/sunyiwu/affinity/xtrimo/openfold\_debug/metrics\_for\_all/openmultimer/notebooks/ecd/ecd\_feature\_process.ipynb

Train data:

/nfs\_baoding\_ai/shaochuan/code/ds\_check/ab\_ag\_training\_v6.csv

/nfs\_baoding\_ai/shaochuan/code/ds\_check/v4\_agabtotal.csv

/nfs\_baoding\_ai/sunyiwu/affinity/xtrimo/openfold\_debug/metrics\_for\_all/openmultimer/notebooks/training\_data/vh\_ag\_training\_v3\_ori

Fasta：

/nfs\_baoding/share/shaochuan/seq/pdb\_seqres.fasta

Pymol:

select binding, byres all within 4.5 of sele

pdbTm:

/nfs\_baoding\_ai/sunyiwu/affinity/xtrimo/openfold\_debug/metrics\_for\_all/openmultimer/notebooks/training\_data/pdbtm\_information.csv

RCSB database：

/pfs\_beijing/share/shaochuan/rcsb\_database/v202307/

Ecm result:

/nfs\_baoding\_ai/sunyiwu/affinity/xtrimo/openfold\_debug/metrics\_for\_all/openmultimer/notebooks/ecd/deeptmhmm\_result/val/

大规模跑程序：

[Kubeflow Central Dashboard (biomap-int.com)](http://mlcpu.biomap-int.com/_/jupyter/new?ns=zhangyan2023)

小规模跑程序：

[Kubeflow Central Dashboard (biomap-int.com)](http://bioflow.biomap-int.com/_/jupyter/?ns=zhangyan2023)

比较结果：

Ground truth：

/nfs\_baoding\_ai/sunyiwu/affinity/xtrimo/openfold\_debug/metrics\_for\_all/openmultimer/notebooks/pdb\_fv159\_ab\_ag\_cut

Predict：

/nfs\_baoding\_ai/sunyiwu/affinity/xtrimo/xtrimo\_docking/differentiable\_rigid\_docking\_infer/openmultimer/model\_test/tune\_opt\_2000

/nfs\_baoding\_ai/shaochuan/code/xtrimo/okr/dev\_epitope/inference/bin/inference/xtrimodock\_output\_10A\_v5\_201\_1.1

Pdb:

Pdbformat

Bio.align:missing\_seq

Wrong:

7kqe, 6opp

/nfs\_baoding/dacheng/B3-process/pdb\_v4/pdb\_reconstruct\_0426/shuffled\_7878\_7kqe.pdb

/nfs\_baoding/dacheng/B3-process/pdb\_v4/pdb\_reconstruct\_0426/shuffled\_3951\_6c6z.pdb

/nfs\_baoding/dacheng/B3-process/pdb\_v4/pdb\_reconstruct\_0426/shuffled\_2621\_5i5k.pdb

/nfs\_baoding\_ai/sunyiwu/affinity/xtrimo/openfold\_debug/metrics\_for\_all/openmultimer/notebooks/pdb\_fv159\_ab\_ag\_cut/7tpj.pdb

**周报：**

**https://web.yammer.com/main/org/biomap.com/groups/eyJfdHlwZSI6Ikdyb3VwIiwiaWQiOiIxMjIwMDk4Nzg1MjgifQ/all**

kubectl get resourceQuota -n shaochuan  
  
 kubectl get pods -n shaochuan

masif 问题记录：<http://git.biomap-int.com:8100/liyakun/bio-masif/-/wikis/home>

masif: http://git.biomap-int.com:8100/liyakun/bio-masif/-/tree/liyakun\_site