# \*ICCPRed: Integrating Unsupervised Language Model with Multi-View Multiple Sequence Alignments for Inter-Chain Contact Prediction\*

This package contains deep learning models and related scripts to run ICCPred.This repository is the official implementation of ICCPred: Accurate prediction of inter-chain contact maps using Integrating unsupervised Language Model with multi-view Multiple Sequence Alignments.

Install virtual environment

conda create -n ICCPred pyhton=3.8

conda activate ICCPred

pip install ESM

#### Extract Multiple Sequence Alignments

cd MSA/

# download library to MSA folder

# <https://zhanggroup.org/cpxDeepMSA/download/package.tar.bz2>

# tar -xvf package.tar.bz2

# mv package/library ../

#

# ls MSA/library

##

python cpxMSA.py -t=targetID -iDir=/home/example

# targetID: target name ie. -t=16gsA-16gsB

# The directory that contains the target directory data. For complexes like 16gsA-16gsB if the directory 16gsA-16gsB full path is /home/user/targets/117eA-117eB the targetpath should store /home/user/targets/ i.e. -iDir=/home/user/targets/

# Extract Feature embedding

Python Extract\_MSA\_Feature\_Embedding.py

# Training ICCPred model

Python train\_single\_model.py

# Testing ICCPred model

Python train\_single\_model.py

test\_model.py