

# 1 Protein Structure Prediction & Ligand Docking 실습

김유빈, 정우엽

2 실습에 들어 가기 전에

# 3

## Download Chimera

- Go to <https://www.cgl.ucsf.edu/chimera/download.html>

### Current Production Releases

3.14.0.10000 (2023-07-10) is the most recent release and also the latest stable release. You can get a copy of any release, but you are more likely to find already installed.

#### 64-bit Releases

Package	Source, Size, and Download	Date	Notes
Windows 64-bit	<a href="#">Download Windows 64-bit</a> Download Windows 64-bit source code	2023-07-10	Runs on Windows 7 or later
Mac OS 64-bit	<a href="#">Download Mac OS 64-bit</a> Download Mac OS 64-bit source code	2023-07-10	Runs on Mac OS 10.14 or later
Linux 64-bit	<a href="#">Download Linux 64-bit</a> Download Linux 64-bit source code	2023-07-10	Compatible on Linux 6.1

64-bit releases are no longer supported:

- Windows 32-bit
- Mac OS 32-bit
- Linux 32-bit

[illegible]

## 5 Modeling Target

6

**Model Protein - 5xra**

**5XRA**  
 Crystal structure of the human 5XRA in complex with agonist (MolProbity DCC: 1.90 Å, R<sub>work</sub> 20.2%, R<sub>free</sub> 23.2%)  
 PDB ID: 5XRA  
 Resolution: 1.90 Å  
 R<sub>work</sub>: 20.2%  
 R<sub>free</sub>: 23.2%  
 a) [PDB](#) | [RCSB PDB](#) | [EMBL-EBI](#) | [PDBe](#)

**5XRA**  
 Crystal structure of the human 5XRA in complex with agonist (MolProbity DCC: 1.90 Å, R<sub>work</sub> 20.2%, R<sub>free</sub> 23.2%)  
 PDB ID: 5XRA  
 Resolution: 1.90 Å  
 R<sub>work</sub>: 20.2%  
 R<sub>free</sub>: 23.2%  
 a) [PDB](#) | [RCSB PDB](#) | [EMBL-EBI](#) | [PDBe](#)

Pharmacophore

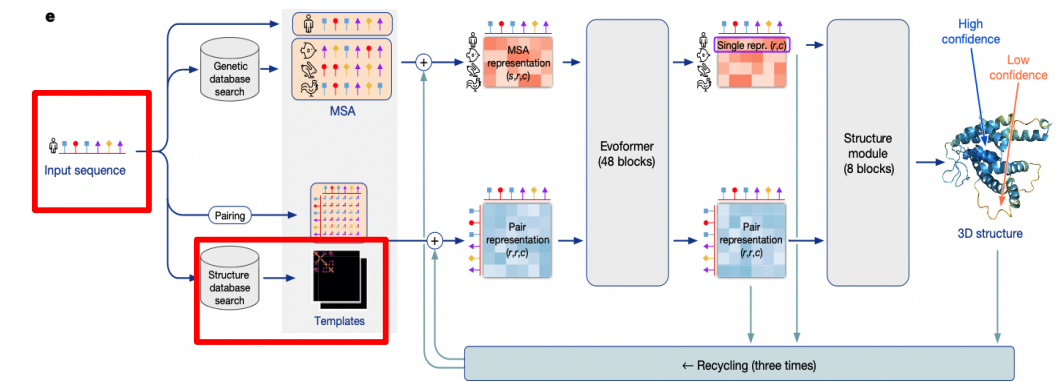
5XRA CB

Agonist AM1542

7

<

# Input Protein sequence



Input protein sequence(s), then hit Runtime -> Run all

**query\_sequence:** "ENFMDIECFMVLNPSQQLAIVLSLTGTFTVLENLLVLCVILHSRSLRCRPSYHFIGSLAVADLLGSVIFVYSFIDFHVHFRKDSRNVFLFKLGGVTASFTASVGSFLAAIDRYISIF"

- Use **:** to specify inter-protein chainbreaks for **modeling complexes** (supports homo- and hetro-oligomers). For example **PI...SK:PI...SK** for a homodimer

```
jobname: "CB1"
```

num\_relax: 5

- specify how many of the top ranked structures to relax using amber

template\_mode: pdb100 

- none = no template information is used. pdb100 = detect templates in pdb100 (see [notes](#)). custom - upload and search own templates (PDB or mmCIF format, see [notes](#))

## 코드 표시

**i) None** - no template information is used

ii) **pd**100**** - detect templates in pd**100** (representative structure database based on the pairwise structure similarity by FoldSeek)

### iii) custom - upload & search own templates

**Chain이 여러 개인 경우 각 chain 사이를 : 로 구분**

**jobname (ex. CB1)**

## Constrained relaxation of structures using Amber force field (stereochemical violation 제거)