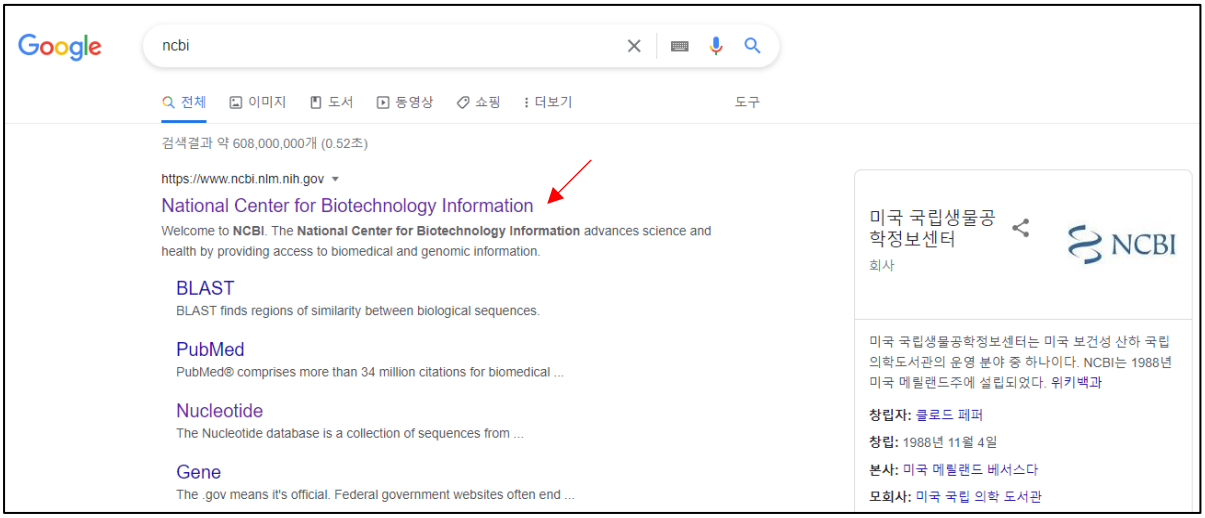
Molecular Biology Laboratory

Bioinformatics and Genomics Lab.

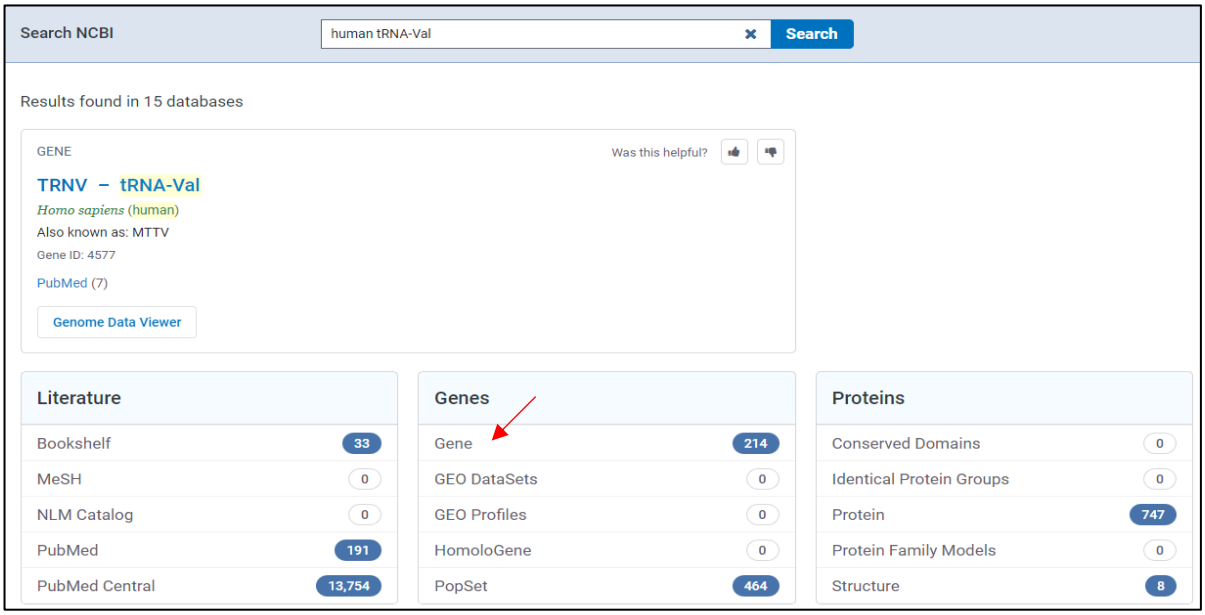
Week3. Structure Prediction of RNA & Proteins

1. Practice how to predict RNA structure

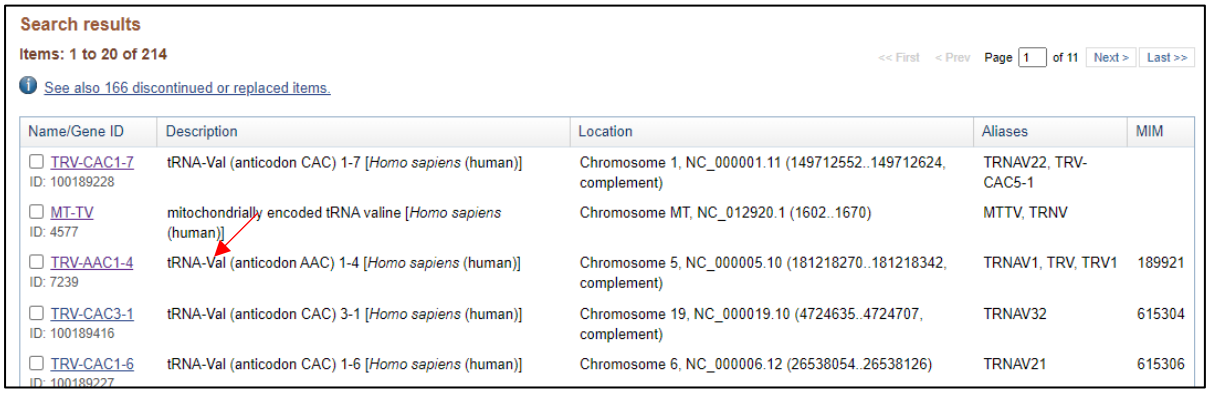
- Predict the structure of "tRNA Val" with "RNAfold" and "mfold"
  - ➢ Search "NCBI" in google and access NCBI.



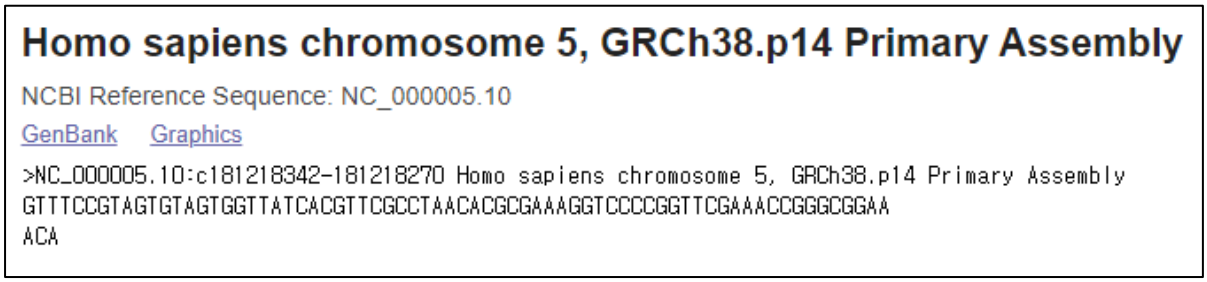
  - ➢ Search "human tRNA-Val" and click "Gene".



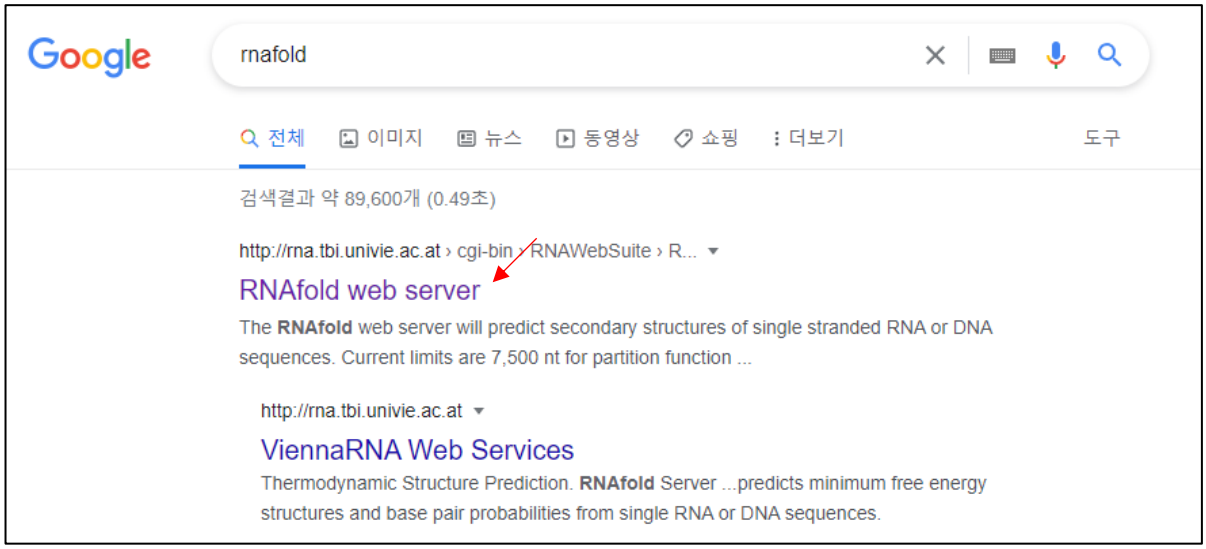
- Select one from the list. We will use 3rd one, "tRNA-Val (anticodon AAC) 1-4" in the practical exercise.



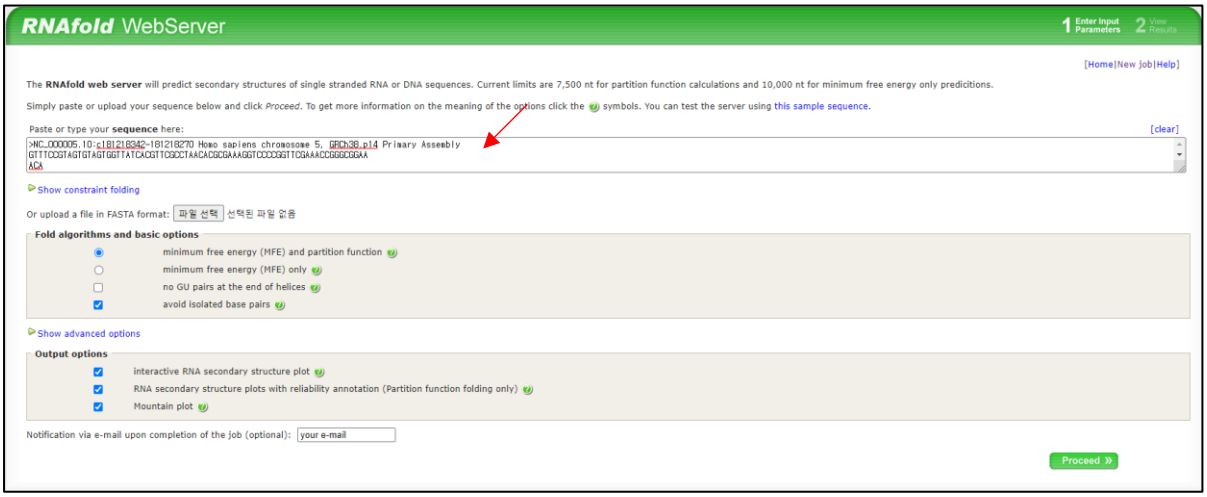
- Click "FASTA" to get the gene sequence of tRNA-Val.



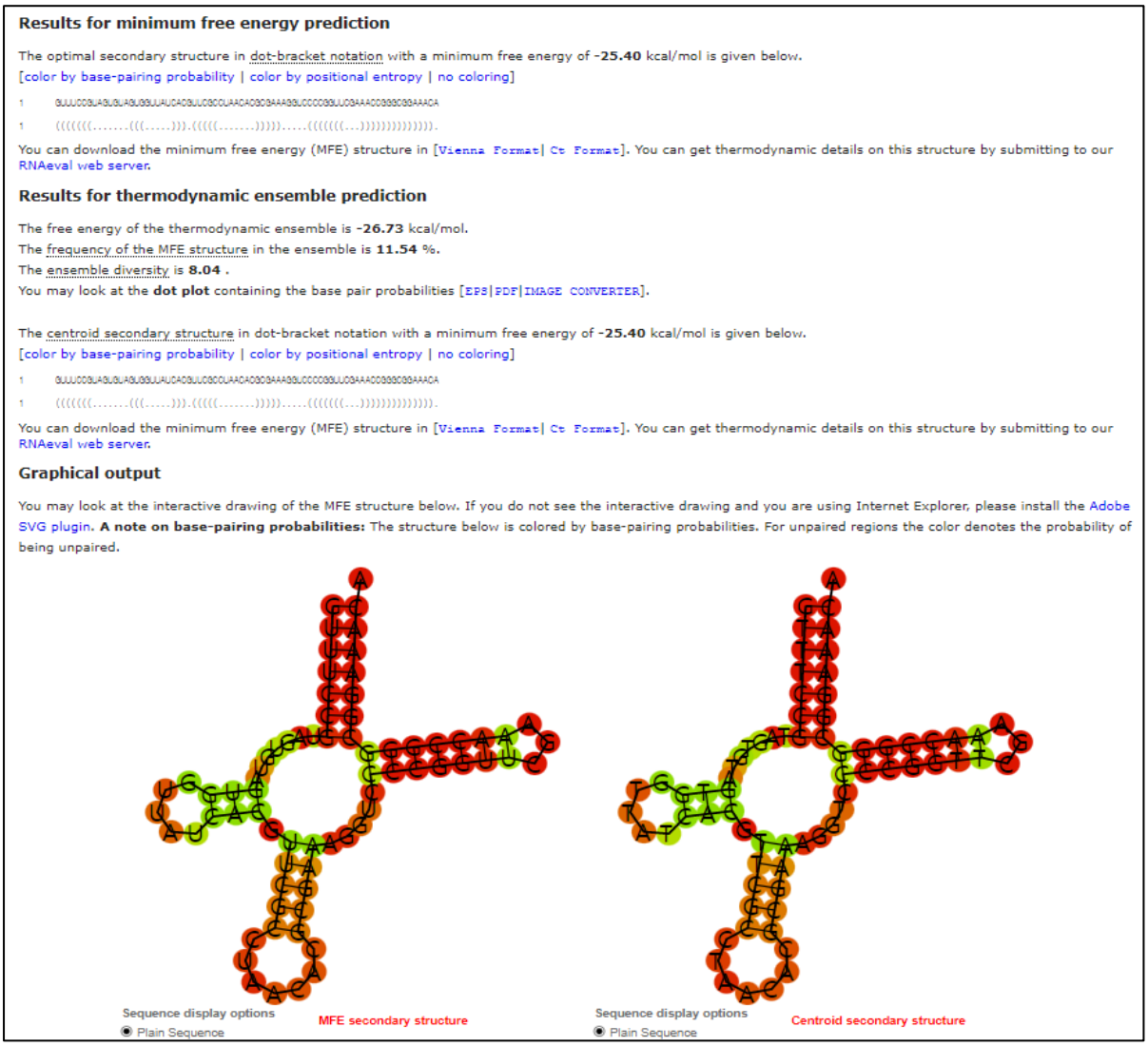
- Search "RNAfold" in google and access RNAfold.



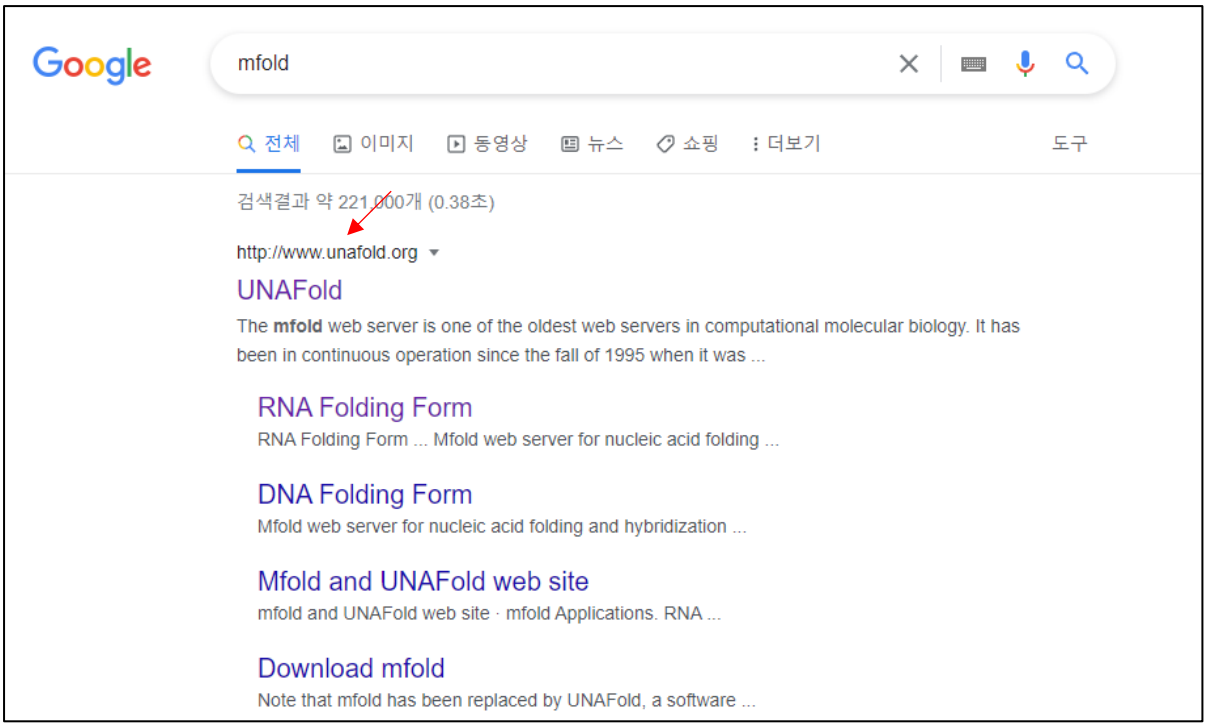
- Copy and paste the tRNA sequence to the box, and click "Proceed" for RNA structure prediction.



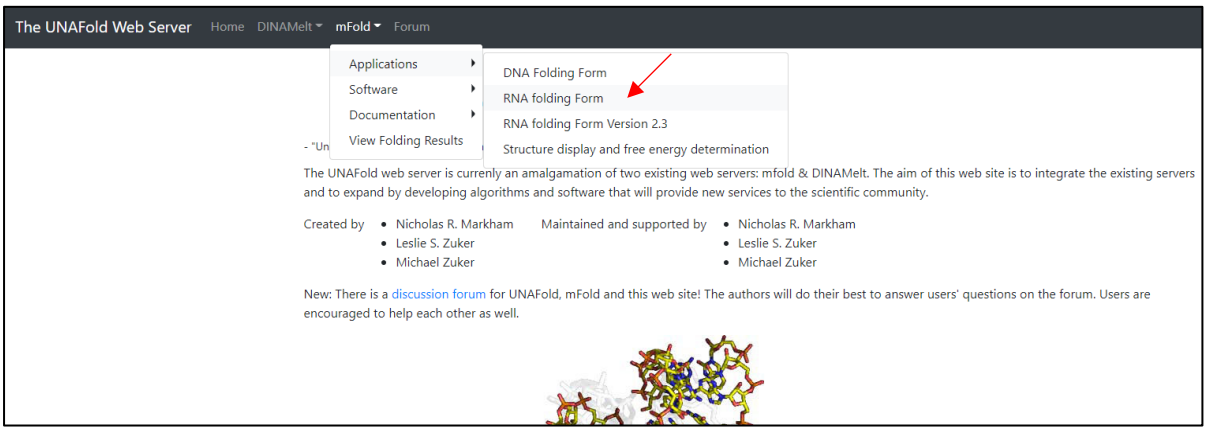
- In the result, we can see the optimal secondary structure of tRNA and its free energy. The left one is the structure that has minimum free energy, and the right one is the structure that has minimum total-base pair distance to all structures in the thermodynamic ensemble.



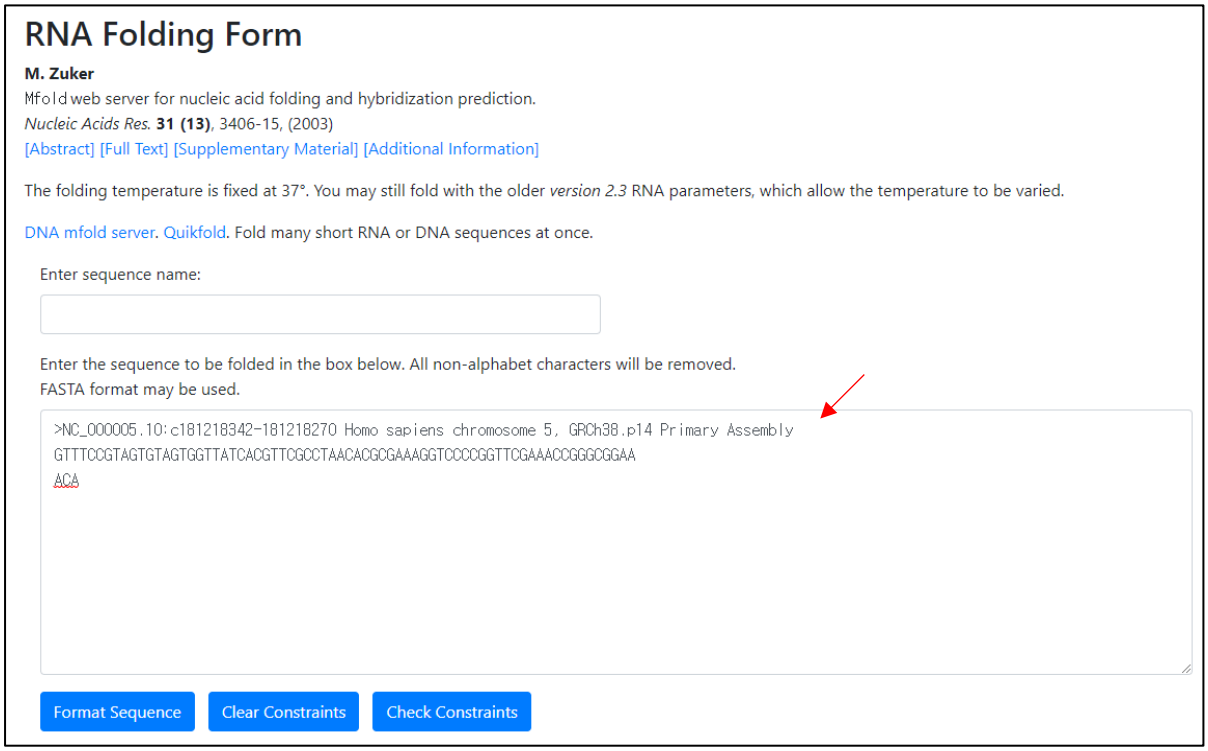
➢ Search "mfold" in google and access UNAfold



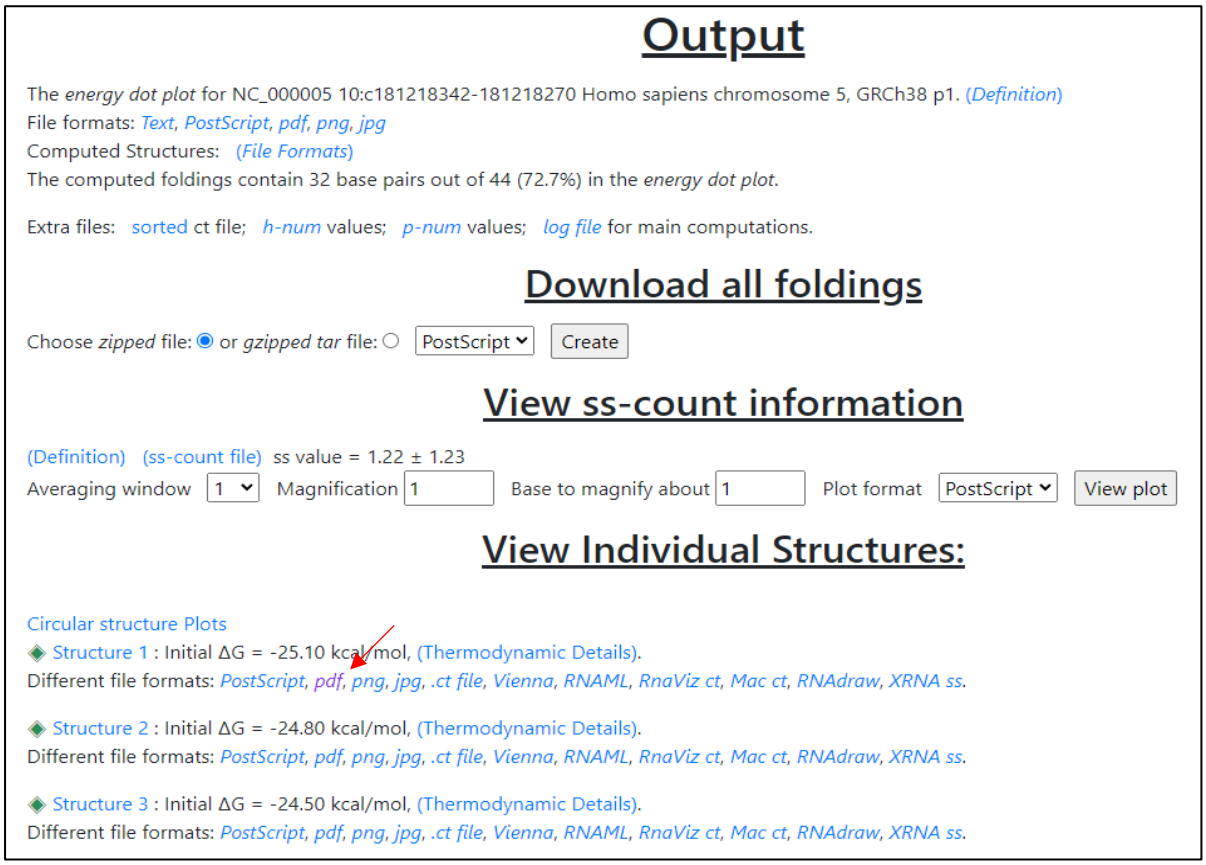
➢ Hover the mouse on the "mFold" - "Applications" and click "RNA folding Form"

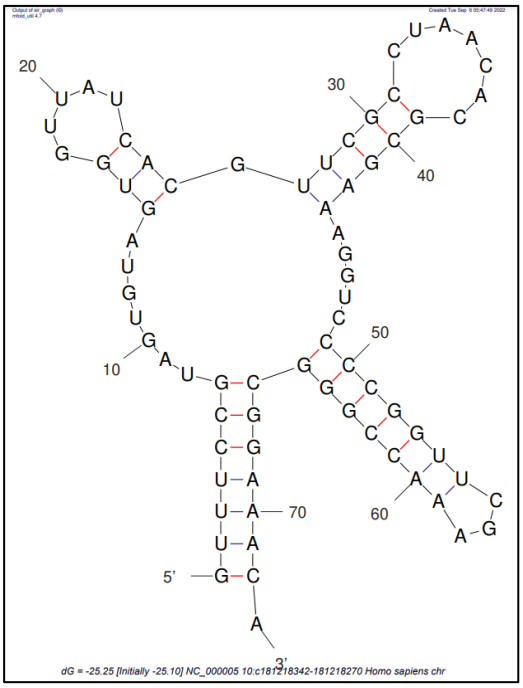


- Copy and paste the tRNA sequence to the box, go to below and click "Fold RNA" for RNA structure prediction.



- In the result, we can see predicted structures and their free energy. Click "pdf" of "Structure 1" then we can see the structure which has minimum free energy




Output of ss_graph (0)
rnlsid_util 4.7
Created Tue Sep 6 00:47:49 2022
20
30
40
10
50
60
70
5'
3'
dG = -25.25 [Initially -25.10] NC_000005 10:c181218342-181218270 Homo sapiens chr

2. Practice how to predict proteins structure

- Predict the structure of green fluorescence protein (GFP) with "PSI-PRED"
  - Go to UniProt and get the protein sequence of GFP

```
>sp|P42212|GFP_AEQVI Green fluorescent protein OS=Aequorea victoria OX=6100 GN=GFP PE=1 SV=1
MSKGEELFTGVVPILVELDGDVNGHKFSVSGEGEGDATYGKLTLKFICTTGKLPVPWPTL
VTTFSYGVQCFSRYPDHMKQHDFFKSAMPEGYVQERTIFFKDDGNYKTRAEVKFEGDTLV
NRIELKGIDFKEDGNILGHKLEYNYNSHNVYIMADKQKNGIKVNFKIRHNIEDGSVQLAD
HYQQNTPIGDGPVLLPDNHYLSTQSALSKDPNEKRDHMVLLEFVTAAGITHGMDELYK
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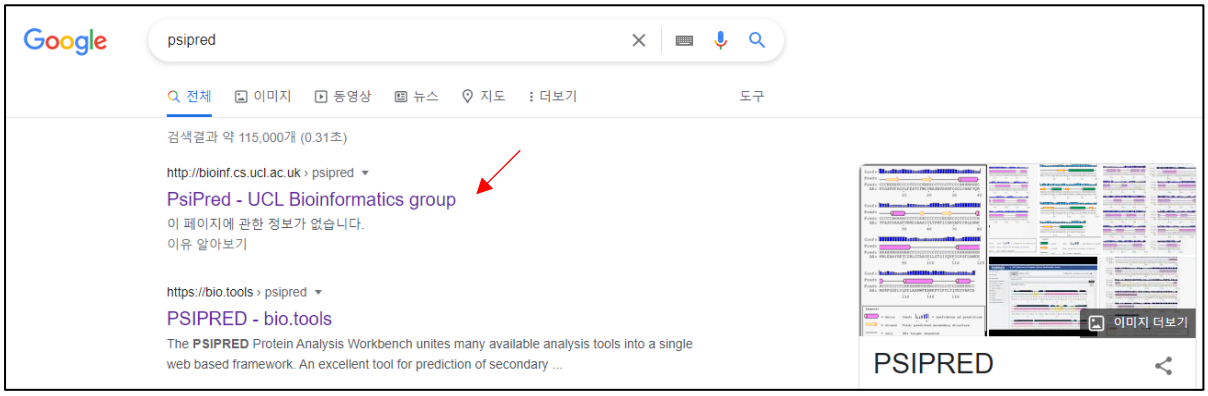
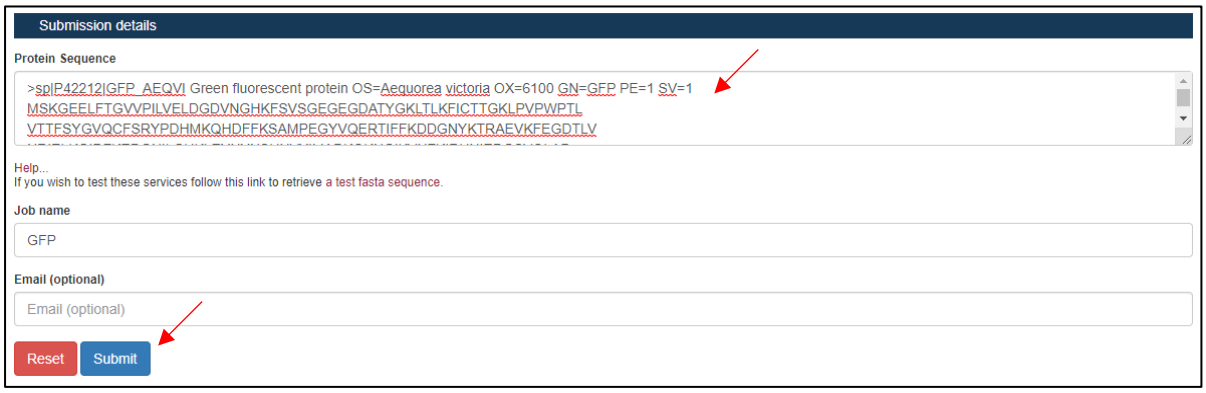
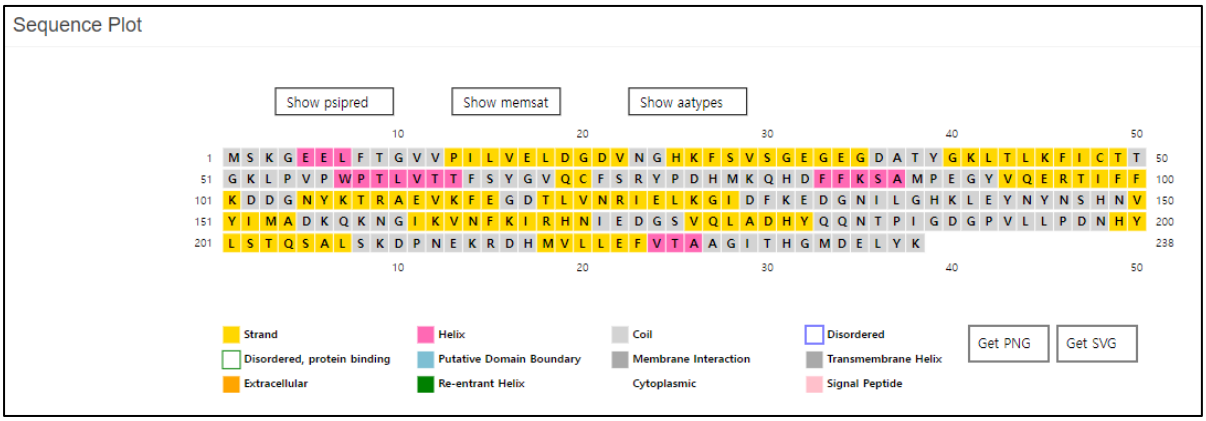
  - Search "psipred" in google and access PSI-PRED.



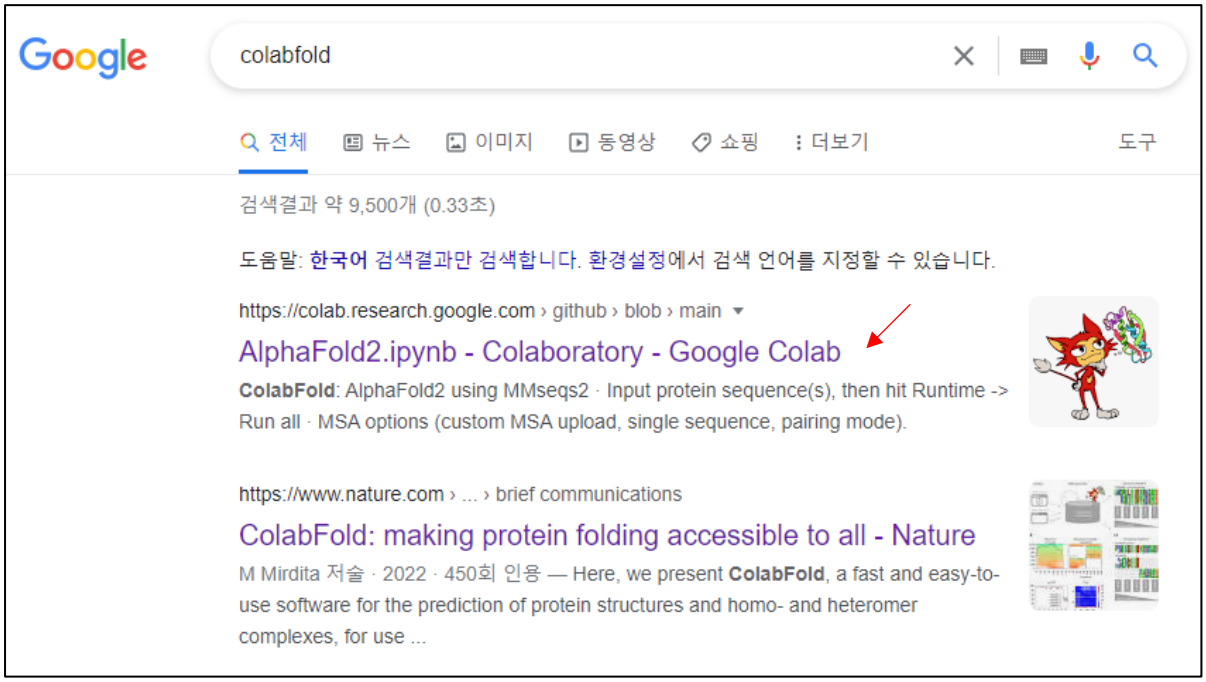
  - Copy and paste the GFP sequence to the box, go to below and click "Submit" for protein secondary structure prediction.



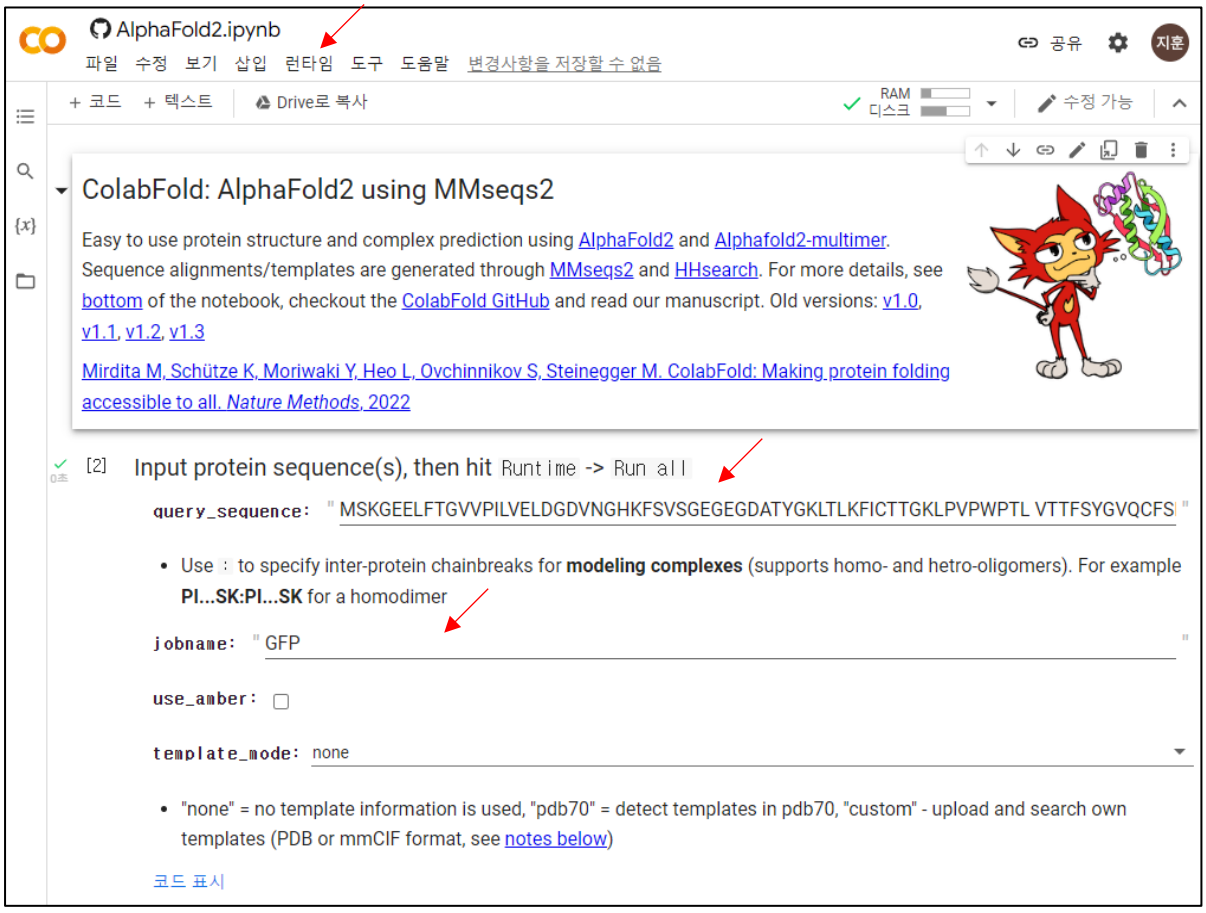
  - In the result, we can separate α-helix, β-sheet, and coil region.



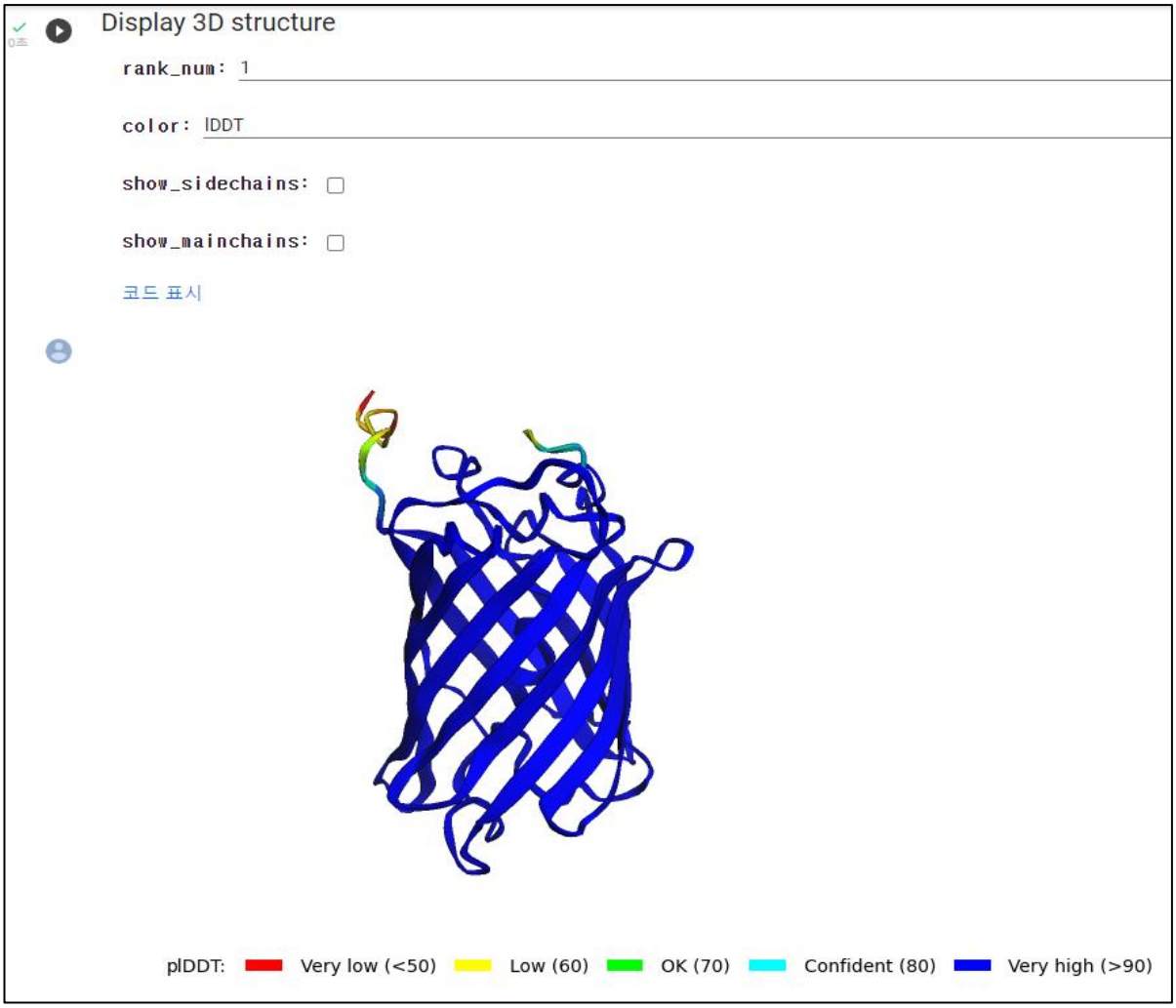
- Predict the 3D structure of GFP and compare with X-ray crystallography image
  - Search "colabfold" in google and access ColabFold.



  - Copy and paste the GFP sequence to the "query_sequence", set job name, and click "Runtime" - "Run all" for protein 3D structure prediction.



- In the result, we can see the 3D structure of GFP.



- Compare the predicted structure and X-ray crystal structure of GFP.