Predicting Peptide Structural Feasibility with CNNs

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Project Goal

Predict the structural feasibility of peptides utilizing CNNs

Motivation

Provide researchers with a predictive tool to accelerate the analysis of peptide model stability.

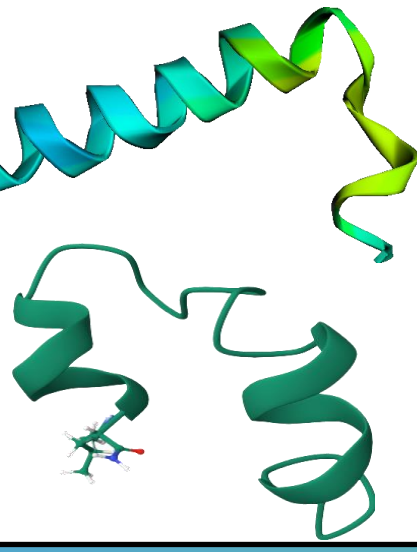
Task 1: Training Set Creation

Create a labeled training set by comparing the structural similarity of generated peptides to their real counterparts

Sequence:
SPLGEEMRDRARAHVDALRTHLAPYS
DELRQRLAARLEALKENGGA

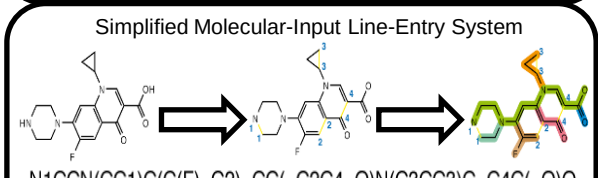
AlphaFold

RCSB PDB PROTEIN DATA BANK



S.M.I.L.E.S

Simplified Molecular-Input Line-Entry System



N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

Adapt Data

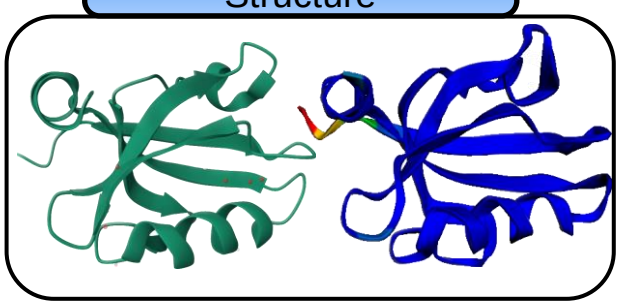
Focus:
- ❑ Reduce Dimensionality
- ❑ Nonadjacent bonding
- ❑ Structural components

.PDB Format

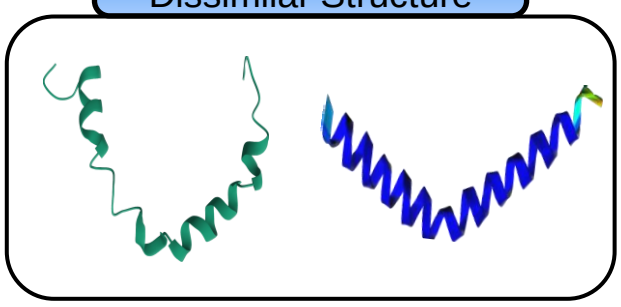
```
ATOM      1  N   HIS B  -1      75.822 -55.481  -8.354  1.00 47.79
ATOM      2  CA  HIS B  -1      76.394 -55.280  -7.029  1.00 57.91
ATOM      3  C   HIS B  -1      76.626 -53.799  -6.752  1.00 52.10
ATOM      4  O   HIS B  -1      77.492 -53.435  -5.956  1.00 47.84
ATOM      5  CB  HIS B  -1      77.707 -56.053  -6.892  1.00 54.37
```

Compare SMILES for Similarity

Positive Label: Similar Structure



Negative Label: Dissimilar Structure



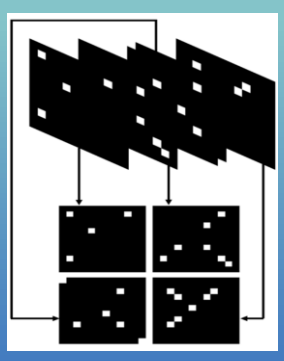
Preliminary Results

Peptide ID:	Cosine Similarity:	Label
Shu3	0.9974	Positive
N7l	0.9913	Positive
e0a	0.2074	Negative
M8l	0.2635	Negative
1CEU	0.3680	Negative
1Hzn	0.4200	Negative
Gw4	0.1675	Negative
1Loi	0.1848	Negative

Future Key Tasks

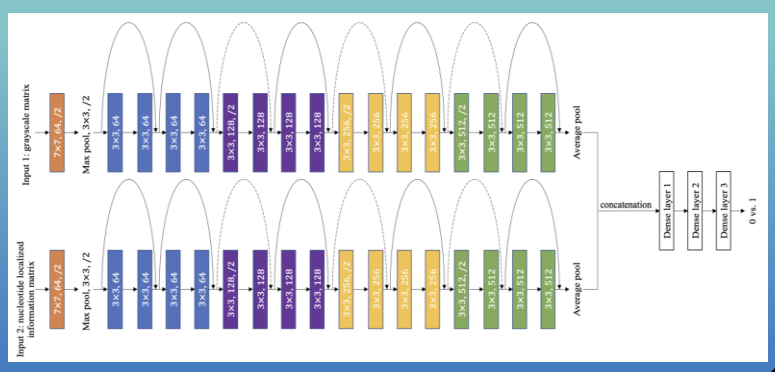
- ❑ **Task 2: Adapt NU-Resnet for Peptide Sequences**

Adapt current RNA based CNN to take in and predict peptide sequences



- ❑ **Task 3: Adapt NUMO-Resnet to utilize Peptide Motifs**

Implement motif input data for NUMO-Resnet CNN to utilize



Sources

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