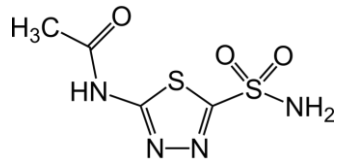**Compound Features**

SMILES

CC(=O)NC1=NN=C(S1)S(N)(=O)=O

C_2

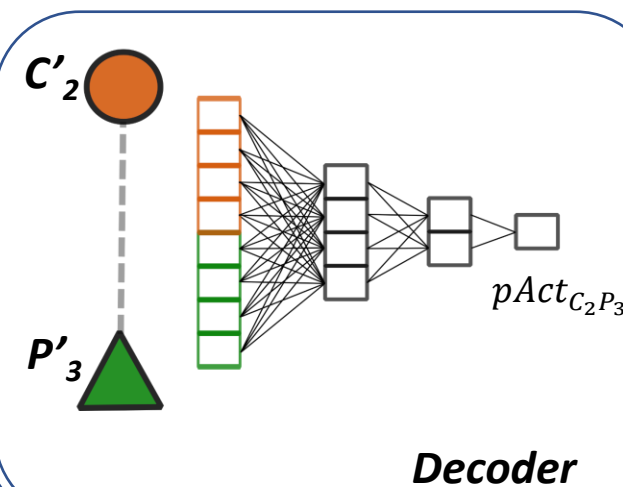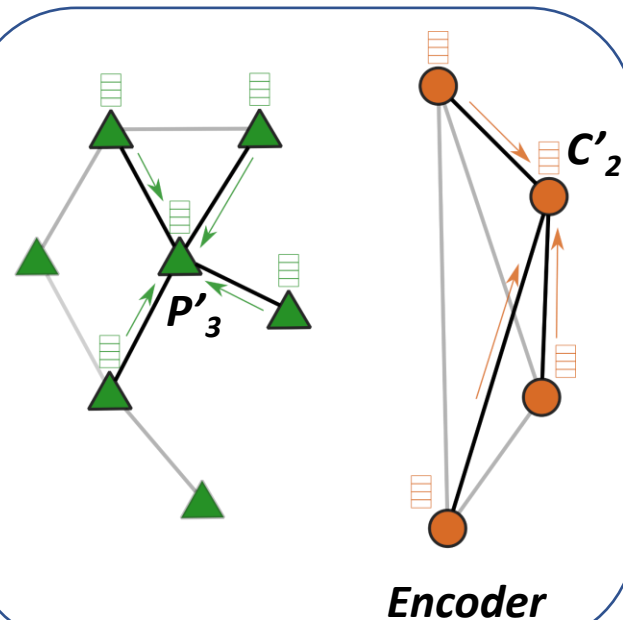**Knowledge Graph**

P_1 P_2
P_5 P_3 P_4
P_6
P_7

C_1
C_2
C_3
C_4

Protein Features

Sequence

SHHWGYG......RQIKASFK

P_3
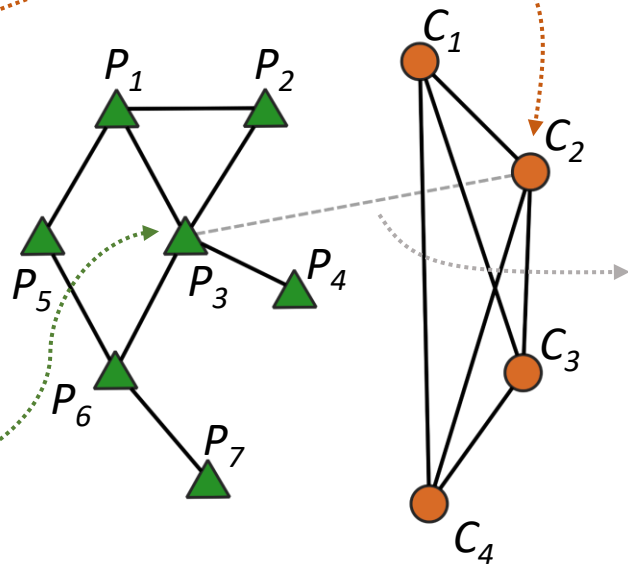
Neural Network Architecture

C'_2

P'_3

Encoder

C'_2

P'_3

$pAct_{C_2P_3}$

Decoder