Polypeptide Helicity and Ensemble Prediction Tool

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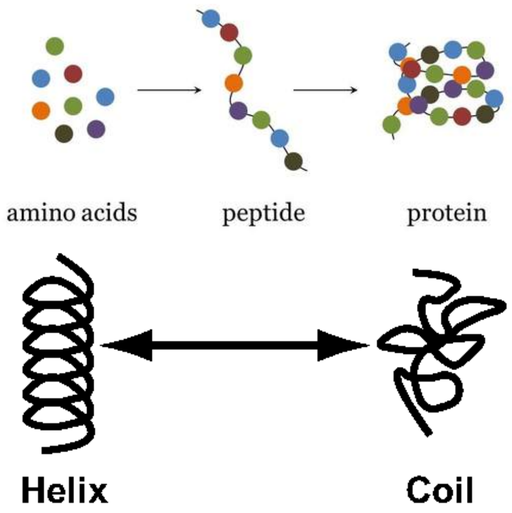
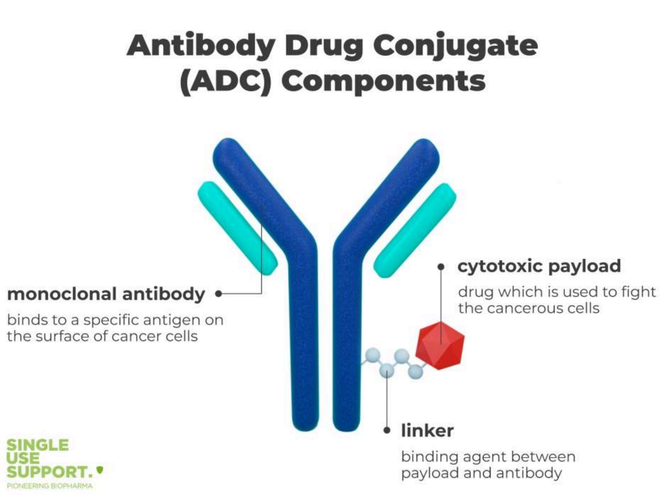
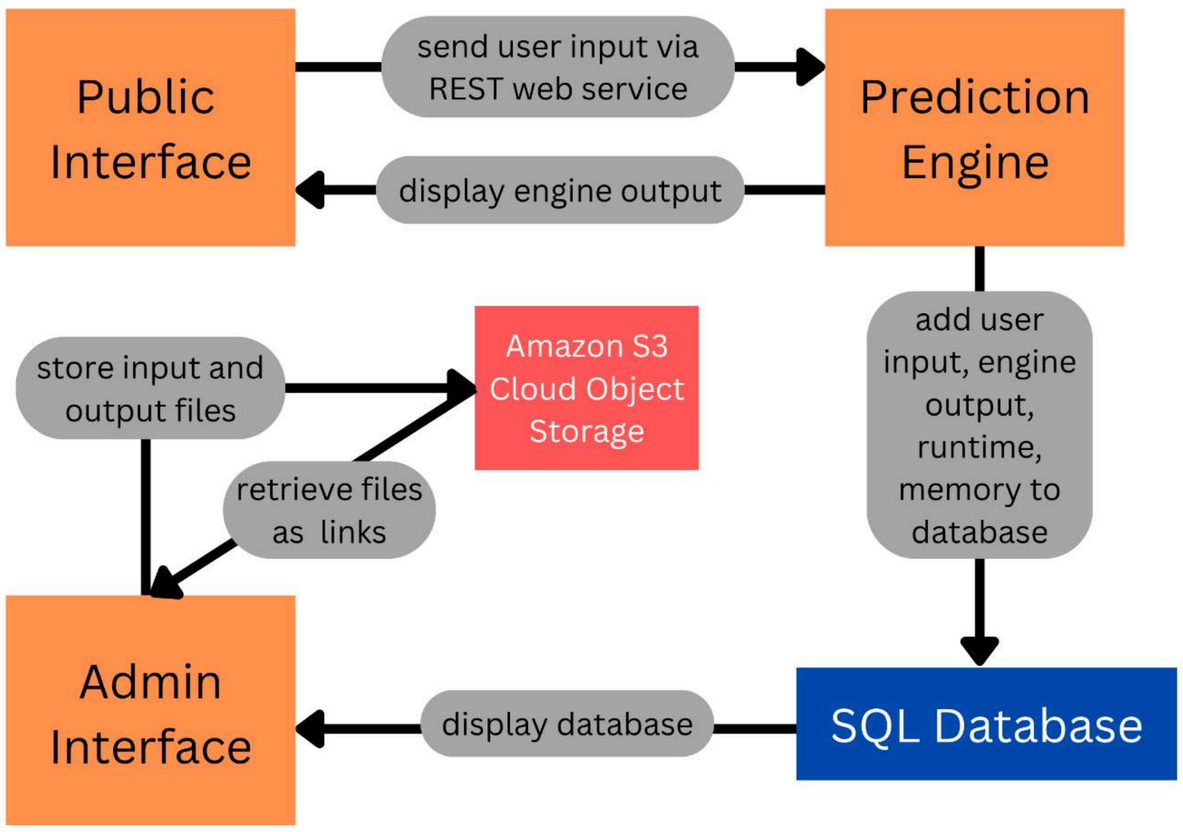
INTRODUCTION & OBJECTIVES

Duke collaborators developed the *Polypeptide Helicity and Ensemble Prediction Tool*, which uses Bayesian statistics to predict the helicity of peptide sequences. Helicity refers to the alpha helix structure on the bottom left. A helical structure is more rigid compared to the coil structure on the right. This tool can help researchers design antibody linkers with the adequate flexibility to target proteins responsible for diseases such as HIV, COVID, and cancer. We built a web application that makes this tool accessible to researchers around the world.





SYSTEM ARCHITECTURE

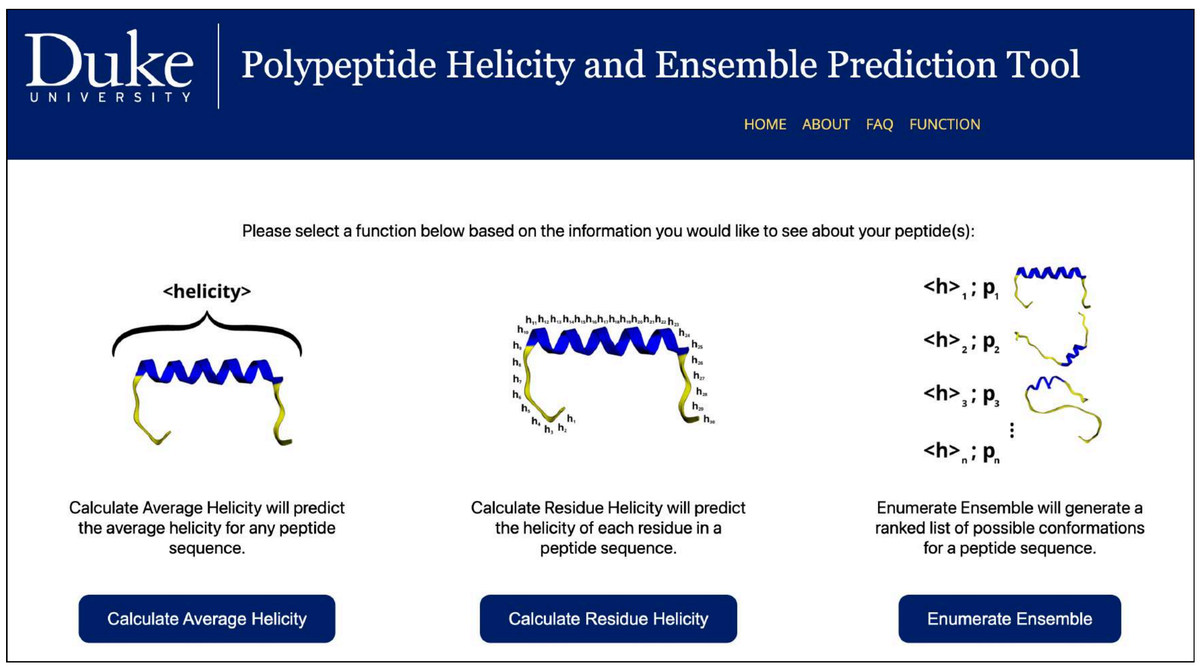


TECH STACK

python · jupyter · PostgreSQL · voilà · FastAPI · GitLab · docker · amazon S3

TOOL FUNCTIONS

CHECK OUT OUR WEBSITE: tinyurl.com/polypeptidewebsite



To receive a prediction, users must submit the following information: sequence, temperature, pH, N-Block, C-Block, urea concentration, and TMAO concentration.

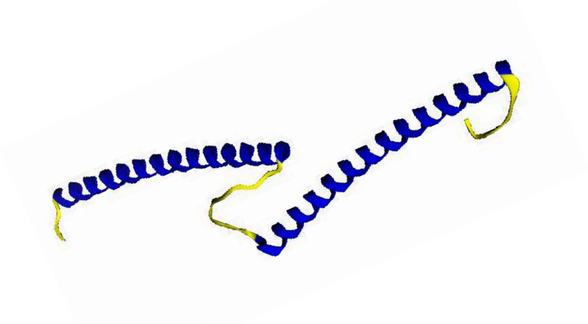
Calculate Average Helicity Function

- Predicts the average helicity for any peptide sequence

sequence	helicity
AAAAQLEDARRLKAIYEKKKNELG	0.137957

Calculate Residue Helicity Function

- Predicts the helicity of each residue in a peptide sequence



A 3D model of the structure is also displayed. This modeling feature is still in beta testing.

residue	sequence	helicity
1	AAAAQLEDARRLKAIYEKKKNELG	0
2	AAAAQLEDARRLKAIYEKKKNELG	0.00586144
3	AAAAQLEDARRLKAIYEKKKNELG	0.00909319
4	AAAAQLEDARRLKAIYEKKKNELG	0.0109083
5	AAAAQLEDARRLKAIYEKKKNELG	0.0117607
6	AAAAQLEDARRLKAIYEKKKNELG	0.118077
7	AAAAQLEDARRLKAIYEKKKNELG	0.10673
8	AAAAQLEDARRLKAIYEKKKNELG	0.285289
9	AAAAQLEDARRLKAIYEKKKNELG	0.238145
10	AAAAQLEDARRLKAIYEKKKNELG	0.204109
11	AAAAQLEDARRLKAIYEKKKNELG	0.185427
12	AAAAQLEDARRLKAIYEKKKNELG	0.205564

Enumerate Ensemble Function

- Generates a ranked list of possible conformations for a peptide sequence

rank	conformation	probability	total_probability	helicity	stat_weight	free_energy
1	ccccccccccccccccccccc	0.348328	0.348328	0	1	-0
2	cccccchccccccccccccc	0.0354122	0.38374	0.0416667	0.101663	1240.09
3	ccccccccccccccccchcc	0.0352536	0.418994	0.0416667	0.101208	1242.53
4	cccccccccccccchccccc	0.0238859	0.44288	0.0416667	0.068573	1453.69
5	ccccccccccccccccccchc	0.022083	0.464963	0.0416667	0.0633971	1496.26
6	cccccccccchccccccccc	0.0182614	0.483224	0.0416667	0.0524258	1599.34
7	cccchccccccccccccccc	0.0152853	0.498509	0.0416667	0.0438818	1695.84
8	ccccccccccccccchcccc	0.0141618	0.512671	0.0416667	0.0406567	1737.25
9	ccccccccccccccccchccc	0.0141618	0.526833	0.0416667	0.0406567	1737.25
10	cccccccccchccccccccc	0.0130945	0.539927	0.0416667	0.0375926	1779.75

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