



## Peptide Optimizer LLM – One-Page Overview

### 1. Project Overview

Built an AI-powered system that predicts optimized peptide sequences for Diabetes, Obesity, and Multiple Sclerosis. The system uses machine-learning models trained on GLP-1 substitution datasets, glatiramer-like peptides, and IL-10/IL-23 immunomodulatory sequences. Users input a peptide sequence, choose a disease, and the system returns Top-K optimized variants with explanations.

### 2. Core Approach

**Diabetes:** GLP-1 potency improvement

**Obesity:** GLP-1 optimization with adaptable scoring

**Multiple Sclerosis:** MS-likeness scoring using glatiramer, IL-10, IL-23 patterns

### 3. ML Models Used GLP-1 Model (Diabetes & Obesity)

**Type:** Random Forest Regressor

**Inputs:** Mutation position, substitution identity

**Output:** GLP1R\_benefit score

### MS Model (Multiple Sclerosis)

**Type:** Random Forest Classifier

**Inputs:** Fraction of A/E/K/Y, hydrophobicity, charge, and length.

**Output:** Probability of MS-likeness

### 4. Optimization Engine

**GLP-1:** Single-point mutants ranked via GLP1R\_benefit.

**MS:** Amino-acid scan mutants ranked via MS-likeness probability.

### 5. Application Architecture

**Frontend:** Streamlit UI

**Backend:** Python optimization engines & ML models

**Deployment:** Hugging Face Spaces (Streamlit runtime)

### 6. Overall Value

Demonstrates how ML + peptide datasets can be used for rapid in-silico therapeutic design, with explainable results.