

BIO ENG C142: Final Project Report (UGRAD)

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April 1, 2025

Abstract

1 Introduction

This project uses the ANI-1 framework. [1]

2 Methods

3 Results

4 Discussion

5 References

1. Smith, J. S., Isayev, O. & Roitberg, A. E. ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost. *Chemical science* **8**, 3192–3203 (2017).