

Improved Generation of Symmetric Cyclic Peptide Complexes with RFdiffusion

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Outline

1. Improved Generation of Symmetric Cyclic Peptide Complexes with RFdiffusion

under the advisory of David Juergens

2. Scaffolding Metal Binding sites

under the advisory of David Juergens, Dr. Gaurav Bhardwaj, Dr. Nikita Hanikel

Guiding Potentials

Factors: intramolecular weights, intermolecular weights

1. weight_intra: 0.7, weight_inter: 0.7
2. weight_intra: 0.8, weight_inter: 0.6
3. weight_intra: 0.5, weight_inter: 0.5
4. weight_intra: 0.8, weight_inter: 0.7

Testing Variances

Factors: guiding decay, number of diffusion steps, guiding scale

1. Guiding decay: linear, quadratic
2. Diffuser steps (T): 16, 20, 25, 35, 50
3. Guiding scale: 0.5, 1, 2, 3, 5 ,8

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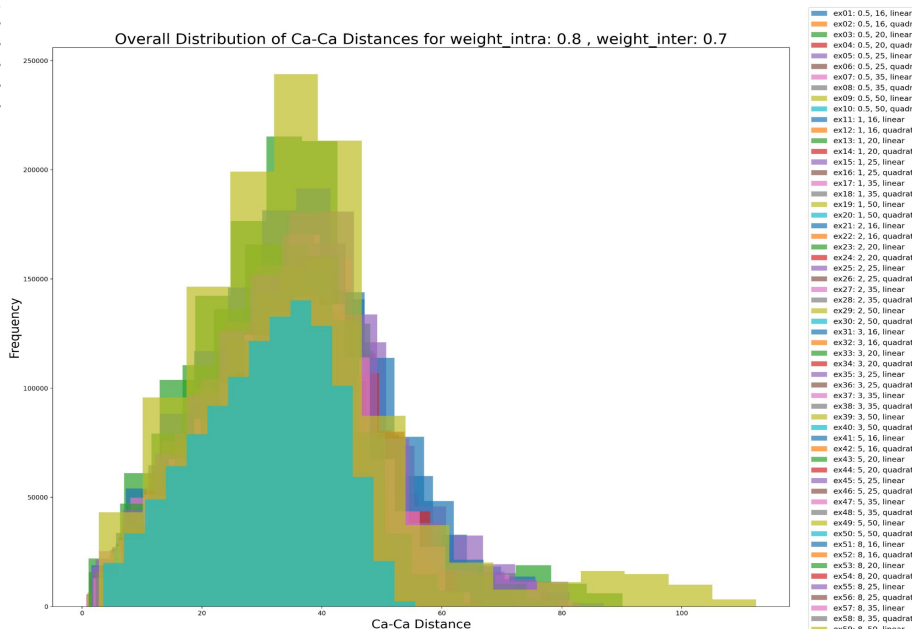
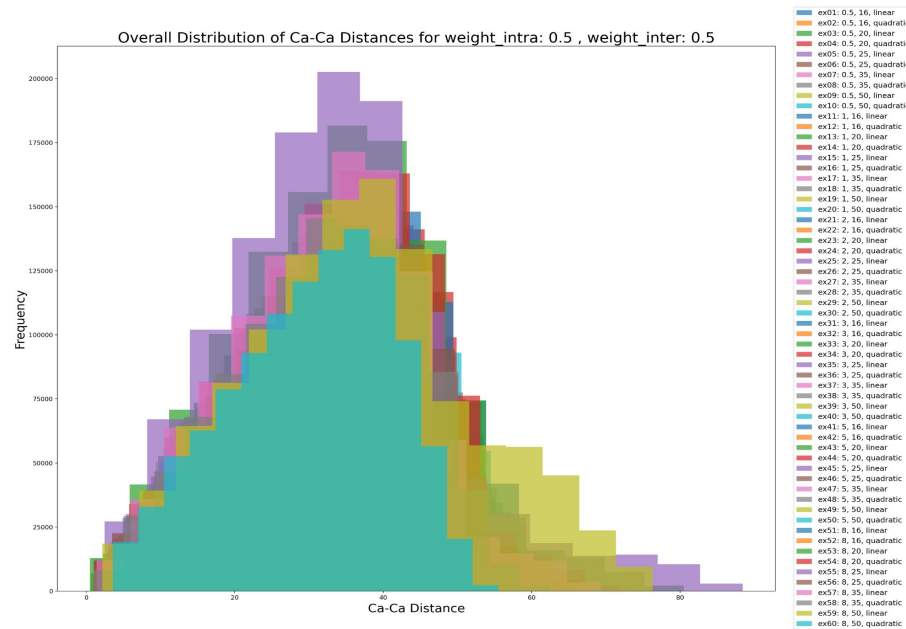
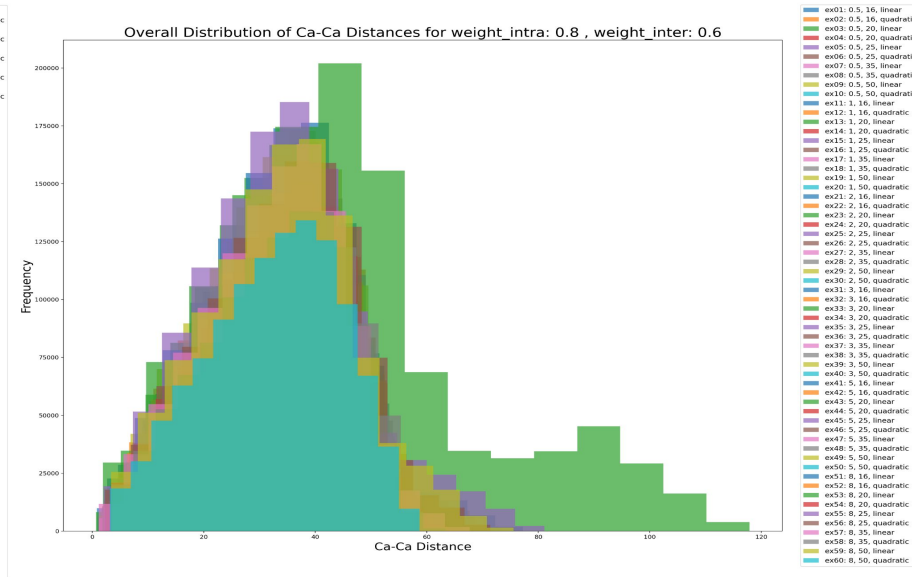
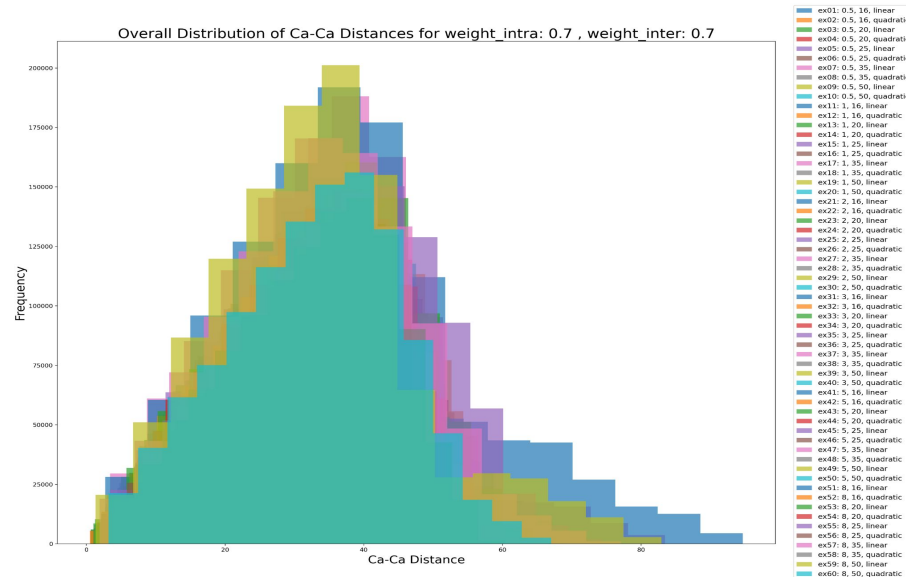
Objective

- This study aims to discover a guiding potential that heavily impacts the overall structure of symmetric oligomers.

Testing Methodology

- For each guiding potential, we displayed the overall distribution of pairwise Ca-Ca distances for the distinctive testing pairs (e.g. Test 1 - 4).
- For same guiding potentials and testing variances with static diffuser steps (e.g. $T=50$), we tested with different number of amino acid chains (e.g. 8, 10, 12, 16, 20 in Test 5-8).

Test 1-4



Test 5-8