Δhelix: Initial Research and Structural License (EN Version)

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1. Background and Purpose

This document outlines the initial design, theoretical framework, and molecular dynamics (MD) evaluation of a newly identified peptide structure termed the **Δhelix** — a compact, self-stabilizing, triangular helical motif derived from resilin. It also defines the usage license for the structure and its derivatives.

2. Definition of Δhelix

The Δhelix is a **novel helical structure not classified as an α-helix or β-sheet**. It exhibits a unique three-sided cross-section, with a helical rotation of approximately **4.5 residues per turn**. According to AlphaFold2 predictions, the spatial arrangement of Cα

atoms describes a twisted triangular form, clearly observable when viewed from above.

3. Structural Design and Characteristics

The Δhelix was first discovered through AlphaFold2 predictions after substituting the terminal glycines (G) in the resilin core peptide (GGRPSDSYGAPGGGN) with threonine (T). These terminal polar residues (T) exhibit **inward hydrogen bonding tendencies**, compressing the central flexible region (rich in G, P, and S residues). This results in a compact, three-dimensional triangular helix formed by physical interactions rather than a hydrogen bond network.

The balance between terminal structural pressure and central flexibility produces a spring-like compressive and restorative behavior.

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4. Representative Δhelix Sequences

The following peptides represent confirmed Δhelix structures:

Δ12（wt） TTRPSDSYGTPTTGN

Δ14（wt） TTRPSDSYGTPTTGNA

Δ30（doubleAS） TTRPSDSYGTPTTGNASTTRPSDSYGTPTTGN

All sequences exhibit stable Δhelix-like folding in AlphaFold2 predictions.

- Stability is further confirmed via molecular dynamics simulations.

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5. MD Simulation Results and Interpretation

Δ14 – 100 ns at Standard Conditions

- **Temperature**: 303.15 K
- **Pressure**: 1 atm
- **Water model**: TIP3P
- **Duration**: 100 ns
- **Engine**: GROMACS 2023

Summary: Δ14 remained stable throughout the simulation. The central core maintained structural integrity while termini showed flexible yet constrained movement. No collapse or misfolding was observed. Structural stabilization was not hydrogen-bond-driven.

Key Metrics:

- **RMSD**: ~0.43 nm, converged early, stable beyond 20 ns
- **Rg**: ~1.05 nm, no major unfolding
- **RMSF**: termini > 0.3 nm, core ~0.1–0.25 nm
- **SASA**: average ~13 nm², central region rolled in
- **Contact map**: mainly i±1, no distant collapse
- **Hydrogen bonds**: minimal (~1/frame), non-persistent
- **PCA**: elastic "twisting" motion along a principal axis
- **End-to-End Distance**: ~2.45 nm, consistently held

Δ 14 – 50 ns under Extreme Conditions (350K, 3 atm)

- **Temperature**: 350.15 K
- **Pressure**: 3 atm
- **Water model**: TIP3P
- **Duration**: 50 ns
- **Engine**: GROMACS 2023

Summary: Even under high temperature and pressure, Δ14 preserved its folded state. The core tightened slightly, and key metrics remained stable. Hydrogen bonding remained minimal, confirming non-covalent compactness as the main stabilizing force.

Key Metrics:

- **RMSD**: ~0.43 nm, stable throughout
- **Rg**: ~1.1 nm, slight compaction
- **RMSF**: termini > 0.3 nm, core ~0.1–0.25 nm
- **SASA**: ~13 nm² average, slight reduction over time
- **Atomic Contacts**: ~7500–8000 per frame, dense and sustained
- **Hydrogen bonds**: ~1.2/frame, not contributing to stability
- **PCA**: deformation limited to elastic twisting
- **End-to-End Distance**: ~2.45 nm, unchanged

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6. Applications and Future Outlook

The Δhelix offers a **previously unknown triangular helical motif** that is compact, hydrogen bond–independent, and self-stabilizing at just ~15 residues. Its properties

suggest potential in:

- **Elastic peptide materials** (e.g., nanoscale springs and sensors)
- **Structural insertion motifs** for fusion proteins (as demonstrated with Δ30 in Trx C-terminal)
- **AI structural prediction training** using Δ14/Δ30 as stable non-canonical folds

Future directions:

- Mutational variants of Δ14
- Higher-order Δ30 polymers
- Structural insertion into compact domains (e.g., WW, GB1)
- Wet-lab synthesis and CD-based confirmation

7. License and Usage Notice

All peptide sequences, structure designs, and theoretical definitions of the Δhelix (including Δ12, Δ14, and Δ30) described in this document are original intellectual products developed and analyzed by the author.

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