

Washington University in St. Louis

Washington University Open Scholarship

Volume 12

Washington University
Undergraduate Research Digest

Spring 2017

Development of an Algorithm to Calculate Torsional Angles of Polypeptide Structures

Krish Tejas Bharat

Washington University in St. Louis

Follow this and additional works at: https://openscholarship.wustl.edu/wuurd_vol12

Recommended Citation

Bharat, Krish Tejas, "Development of an Algorithm to Calculate Torsional Angles of Polypeptide Structures" (2017). *Volume 12*. 15.

https://openscholarship.wustl.edu/wuurd_vol12/15

This Abstracts A-I is brought to you for free and open access by the Washington University Undergraduate Research Digest at Washington University Open Scholarship. It has been accepted for inclusion in Volume 12 by an authorized administrator of Washington University Open Scholarship. For more information, please contact digital@wumail.wustl.edu.

DEVELOPMENT OF AN ALGORITHM TO CALCULATE TORSIONAL ANGLES OF POLYPEPTIDE STRUCTURES

Krish Tejas Bharat

Mentor: Rohit Pappu

Dihedral angles ϕ (phi) and ψ (psi) are important structural factors that determine local conformations of peptides. As a part of an effort to assess ϕ - ψ angle distributions within amino acid motifs known as short linear motifs (SLiMs) found in intrinsically disordered regions (IDRs) that are implicated in diseases such as Alzheimer's disease and Mad Cow disease, this study reports the development of a tool to calculate torsional angles of given polypeptide structures. From a trajectory file generated by a molecular simulation software, the algorithm generates ϕ - ψ angle distributions at different time points along the length of a simulation. To illustrate its application, we used OpenMM, a molecular simulation package, to run molecular dynamics simulations on various dipeptide chains, and parsed dihedral angles to obtain ϕ - ψ distributions for different systems.