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(G) (POS-34) A Computational Study on the Structural Dependence of Cell Penetrating Peptide Pathways

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<h1> A Computational Study on the Structural Dependence of Cell Penetrating Peptide Pathways </h1>

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 Cell penetrating peptides (CPPs) are group of short sequence peptides with the intrinsic ability to drive internalization into the cellular membrane[1,3,4]. CPPs may internalize through a energy independent processes (direct penetration) or energy dependent processes (endocytosis)[1,3,4]. The cellular uptake method of CPPs is poorly understood on a case by case basis due to the vast possible factors that may alter the uptake mechanism. Molecular Dynamics (MD) has been used successfully to study the behavior of CPPs, however, due to internalization happening on timescales not accessible with conventional MD, sampling methods or coarse graining must be applied[2]. In this study, the structural dependence of the internalization pathway of CPPs is examined with a constant membrane composition. MD coupled with replica exchange molecular dynamics (REMD) is applied to study a model CPP. The structure of the CPP is varied via cyclization and sequence modification. Novel analysis techniques are used along with conventional analysis to disseminate the structural factors which effect the internalization of CPPs.

[1] Trofimenko, et al., Genetic, cellular, and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore, eLife, 2021
[2] Lima, et al., Biological Membrane-Penetrating Peptides: Computational Prediction and Applications, Front. Cell. Infect. Microbiol., 2022
[3] Bereau, et al., Folding and Insertion Thermodynamics of the Transmembrane WALP Peptide., J. Chem. Phys., 2015.
[4] Pourmousa, et al., Molecular Dynamic Studies of Transportan Interacting with a DPPC Lipid Bilayer. J. Phys. Chem. B, 2013.

Keyword-1

Cell Penetrating Peptide

Keyword-2

Molecular Dynamics

Keyword-3

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