

RESEARCH

Interactive Exploration of Ligand Movements through Multiscale Temporal Tunnels

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References

Abstract

Background: TODO BK

Results: TODO BK

Conclusions: TODO BK

Keywords: Molecular Sequence Analysis; Molecular Structural Biology; Computational Proteomics

Background

TODO BK + JP (Intro + RW)

Method

Overview + workflow - BK

Trajectory Simplification - AJ

Including mathematical model.

Derivation of Attributes - JB

ligand attributes + attributes of its surrounding

Temporal Tunnel - JB

Visual Exploration

Data Views - BK + ladies

motivation, design

3D, bar charts, scatterplot

Analysis Procedure - BK, JP

Results and Discussion - BK

use case + feedback

Conclusions - All

and future work

Competing interests

The authors declare that they have no competing interests.

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