
MDSCAN

Release 0.0.1

Roy Gonzalez-Aleman

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WHY MDSCAN ?

1.1 How Does MDSCAN Works ?

1.2 Performance Benchmark

1.3 Useful Alternatives

INSTALLATION

2.1 MDTraj

2.2 MDSCAN

2.3 VMD and VMD clustering plugin (optional)

TECHNICAL REFERENCE

3.1 Arguments in Details

3.2 Syntax Selection Examples

3.3 Visualizing Clusters in VMD

CASE STUDY TUTORIALS

4.1 Clustering a MD

4.2 Clustering a Docking Ensemble

CHAPTER

FIVE

LICENSE

CITATION

Complete after academic publication.

VERSION 0.0.1

First version. This corresponds to what is described in the academic publication.

FREQUENTLY ASKED QUESTIONS

8.1 Q1: Does MDTRAJ always align trajectory?

Well ... yep!