The Journal of Open Source Software

# MSMExplorer: Data Visualizations for Biomolecular Dynamics

**Carlos X. Hernández**[1], **Matthew P. Harrigan**[1], **Mohammad M. Sultan**[1], **and Vijay S. Pande**[1]

**1** Stanford University

**DOI:** 10.21105/joss.00188

**Software**

- Review
- Repository
- Archive



## Summary

*MSMExplorer* is a Python package for visualizing data generated from biomolecular dynamics. While molecular visualizations have been a large focus of the molecular dynamics (MD) community (Humphrey, Dalke, and Schulten 1996, Schrödinger, LLC (2015)), data visualizations for the analyses of MD trajectories have been less developed. *MSMExplorer* seeks to fill this niche by providing publication-quality statistical plots with an easy-to-use Python API that works seamlessly with commonly used Python libraries, such as `numpy` and `scikit-learn` (Walt, Colbert, and Varoquaux 2011, Pedregosa et al. (2011)). Additionally, plots are generated using already established plotting libraries, like `seaborn`, to provide a consistent aesthetic (Waskom et al. 2016, Hunter (2007), Hagberg, Schult, and Swart (2008), Foreman-Mackey (2016)).

Plotting functionality in *MSMExplorer* is centered around the statistical tools available in `msmbuilder` (M. P. Harrigan et al. 2017). Because of this focus, in addition to standard time-series plots, users can choose to plot more involved measures, such as Gibbs free energy and implied timescales estimated from Markov models.

*MSMExplorer* is actively developed and maintained by researchers at Stanford University. Source code for *MSMExplorer* is hosted on GitHub and is continuously archived to Zenodo (C. Hernández, Harrigan, and Pande 2016). Full documentation, including a practical example gallery, can be found at http://msmbuilder.org/msmexplorer.

## References

Foreman-Mackey, Daniel. 2016. "Corner.py: Scatterplot Matrices in Python." *The Journal of Open Source Software* 1 (2). The Open Journal. doi:10.21105/joss.00024.

Hagberg, Aric A., Daniel A. Schult, and Pieter J. Swart. 2008. "Exploring Network Structure, Dynamics, and Function Using NetworkX." In *Proceedings of the 7th Python in Science Conference (Scipy2008)*, 11–15. Pasadena, CA USA.

Harrigan, Matthew P., Mohammad M. Sultan, Carlos X. Hernández, Brooke E. Husic, Peter Eastman, Christian R. Schwantes, Kyle A. Beauchamp, Robert T. McGibbon, and Vijay S. Pande. 2017. "MSMBuilder: Statistical Models for Biomolecular Dynamics." *Biophysical Journal* 112 (1): 10–15. doi:10.1016/j.bpj.2016.10.042.

Hernández, Carlos, Matthew Harrigan, and Vijay Pande. 2016. "Msmexplorer/Msmexplorer: MSMExplorer 0.3." doi:10.5281/zenodo.162942.

Humphrey, William, Andrew Dalke, and Klaus Schulten. 1996. "VMD – Visual Molecular

Dynamics." *Journal of Molecular Graphics* 14: 33–38.

Hunter, J. D. 2007. "Matplotlib: A 2d Graphics Environment." *Computing in Science & Engineering* 9 (3). IEEE COMPUTER SOC: 90–95. doi:10.1109/MCSE.2007.55.

Pedregosa, F., G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, et al. 2011. "Scikit-Learn: Machine Learning in Python." *Journal of Machine Learning Research* 12: 2825–30.

Schrödinger, LLC. 2015. "The PyMOL Molecular Graphics System, Version 1.8."

Walt, Stéfan van der, S Chris Colbert, and Gael Varoquaux. 2011. "The NumPy Array: A Structure for Efficient Numerical Computation." *Computing in Science & Engineering* 13 (2): 22–30. doi:10.1109/MCSE.2011.37.

Waskom, Michael, Olga Botvinnik, drewokane, Paul Hobson, David, Yaroslav Halchenko, Saulius Lukauskas, et al. 2016. "Seaborn: V0.7.1 (June 2016)." doi:10.5281/zenodo.54844.