

Manubot Rootstock: Molecular motors with barriers

Authors

- **Daniel S. Himmelstein**
[0000-0002-3012-7446](#) · [@dhimmel](#) · Department of Systems Pharmacology and Translational Therapeutics, University of Pennsylvania · Funded by GBMF4552
- **Anthony Gitter**
[0000-0002-5324-9833](#) · [@agitter](#) · Department of Biostatistics and Medical Informatics, University of Wisconsin-Madison and Morgridge Institute for Research · Funded by NIH U54AI117924
- **Venkat S. Malladi**
[0000-0002-0144-0564](#) · [@vsmalladi](#) · The Laboratory of Signaling and Gene Expression, Cecil H. and Ida Green Center for Reproductive Biology Sciences, University of Texas Southwestern Medical Center

Abstract

TBD

Outline

1. Surface with and without a barrier
2. Family of curves showing force on the barrier as a function of height and position of the barrier.
3. Optimization of a surface for flux and force with and without a barrier. [[1](#)]

Ideas

1. MD and umbrella sampling of a Feringa-type motor.

2. pH change can be modeled as a change in substrate concentration, for our purposes.
 3. Can the experimental groups synthesize motors based on an energy surface?
 4. CD can be a platform -- a scaffold -- for building, but it will be hard to figure out the appropriate assays.
1. Slochower DR, Wang Y-H, Tourdot RW, Radhakrishnan R, Janmey PA. 2014 Counterion-mediated pattern formation in membranes containing anionic lipids. *Advances in Colloid and Interface Science***208**, 177–188. See <https://doi.org/10.1016/j.cis.2014.01.016>.