

Availability of data and materials – raw molecular dynamics (MD) simulation data is too large to deposit online (20 terabytes) but can be made available network to network upon request to GAB. NOTE: data transfer may take several weeks over WiFi. The simulation software is available on GitHub and the DROIDS 3.0 software landing website. For researchers looking to replicate findings, it might be easier to regenerate the study using the PDB structures reported and software provided, rather than transfer the data and generate trajectories one at a time. Because we use an ensembling approach to MD, several hundreds of initiating points in the simulations are generated randomly, and thus there are several hundred MD control, topology, and coordinate files as well.

DROIDS 3.0 requires an Amber18 license, and freely available R install and UCSF Chimera software built upon a Debian Linux desktop distribution or Virtual Machine (VM). Instructions for running on Windows using VirtualBox or Google Cloud Platform VM are provided.

The software, software installer, user manual and tutorial can be accessed at the promotional website and GitHub repository links below

<https://people.rit.edu/gabsbi/>

<https://github.com/gbabbitt/DROIDS-3.0-comparative-protein-dynamics>