**Implementation of Bacilliform Viral Capsid Models**

Daniel Antonio Negrón, PhD1

1Bioinformatics and Computational Biology Program, School of Systems Biology, George Mason University, 10900 University Blvd, Manassas, Virginia 20110, USA

The democapsid application is an interactive, browser-based tool for designing accurate three-dimensional models of icosahedral viral capsids and exporting them to SVG, which is an infinitely scalable format compatible with widely available office-productivity software. This allows the user to easily edit the model without losing quality. Thus, the goal is to aid in the design of publication-quality diagrams to communicate results in molecular biology and nanotechnology. Initially, the code implemented Caspar-Klug Theory (1), which defines a method for the construction of icosahedral capsids. It is based on a parameterized walk over a hexagonal unit lattice, which starts by moving *h* units forward, turning 60 degrees (levo or dextro), and moving *k* units forward until a triangular face is carved. An additional step arranges the face into an icosahedron. Moody extended this model to account for bacilliform phages with fivefold symmetry (2). Here, an updated version of democapsid is presented based on results from Luque and Reguera, whose work generalized the models of Caspar, Klug, and Moody for elongated capsids with fivefold, threefold, and twofold symmetry (3). Additional methods were developed to realize the corresponding three-dimensional structures and described here. The implementation is also consistent with the work of Twarock and Luque, which provides additional Archimedean lattices models (4). Free and open source code is available at <https://github.com/dnanto/democapsid> under the MIT License and the application is available at <https://dnanto.github.io/democapsid/capsid.html>.

Thank you to my committee chair Dr. Donald Seto and co-chairs Dr. Patrick Gillevet and Dr. Sterling Thomas.

1. Caspar DL, Klug A. Physical principles in the construction of regular viruses. Cold Spring Harb Symp Quant Biol. 1962;27:1–24.

2. Moody MF. The shape of the T-even bacteriophage head. Virology. 1965 Aug 1;26(4):567–76.

3. Luque A, Reguera D. The Structure of Elongated Viral Capsids. Biophys J. 2010 Jun 16;98(12):2993–3003.

4. Twarock R, Luque A. Structural puzzles in virology solved with an overarching icosahedral design principle. Nature Communications. 2019 Sep 27;10(1):4414.