

Supplementary

Materials

Integrating Conformational Dynamics and Perturbation-Based Network Modeling for Mutational Profiling of Binding and Allostery in the SARS-CoV-2 Spike Variant Complexes with Antibodies: Balancing Local and Global Determinants of Mutational Escape Mechanisms

Gennady Verkhivker,^{1,2*} Steve Agajanian¹, Ryan Kassab¹, Keerthi Krishnan¹

¹ Keck Center for Science and Engineering, Graduate Program in Computational and Data Sciences, Schmid College of Science and Technology, Chapman University, Orange, CA 92866, United States of America

² Department of Biomedical and Pharmaceutical Sciences, Chapman University School of Pharmacy, Irvine, CA 92618, United States of America

*Correspondence: verkhivk@chapman.edu; Tel.: +1-714-516-4586 (G.V)

Supplemental Materials include scripts for computation of distance fluctuations from MD simulations.