Non-equilibrium Protein Complexes as Molecular Automata

Jan Kocka,[1] Kabir Husain,[1,2,*] and Jaime Agudo-Canalejo[1,*]

[1] *Department of Physics and Astronomy, University College London, London WC1E 6BT, United Kingdom*
[2] *Laboratory for Molecular Cell Biology, University College London, London WC1E 6BT, United Kingdom*

Considerable effort is being put into understanding how biological and biomimetic systems store and process information, a field known as molecular computation. Here we build a thermodynamically consistent kinetic model of a molecular complex made of identical subunits which can be in one of two states (e.g., phosphorylated or not). We then analyse the dynamics of the complex when each subunit can be modified by driven enzymes which act conditionally based on the state of its neighbours. For strongly driven enzymes we identify a one-to-one mapping to elementary cellular automata rules, each rule corresponding to a set of up to eight enzymes. Among these rules we find a rich set of behaviours, including multistability and dynamical steady states. Finally, we show how to deterministically manipulate the state of the complex by sequentially changing the rule (i.e. which enzymes are present) and map out the error-correcting capabilities of different steady states.

* These authors contributed equally. Email: kabir.husain@ucl.ac.uk, j.agudo-canalejo@ucl.ac.uk