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*What Do Molecules Do When We're Not Looking? State Sequence Analysis for Stochastic Chemical Systems*

Many biomolecular systems depend on orderly sequences of chemical transformations or reactions to carry out their functions. Yet, the dynamics of single molecules or small-copy-number molecular systems are significantly stochastic. I will describe State Sequence Analysis, a new approach for predicting or visualizing the behaviour of stochastic molecular systems by computing maximum probability state sequences based on initial conditions or boundary conditions. I demonstrate this approach by analyzing the acquisition of drug-resistance mutations in the HIV genome, which depends on rare events occurring on the timescale of years, and the stochastic opening and closing behaviour of a single sodium ion channel, which occurs on the timescale of milliseconds. In both cases, the approach yields novel insights into the stochastic dynamical behaviour of these systems, including insights that are not correctly reproduced in standard time-discretization or stochastic-simulation approaches to trajectory analysis.