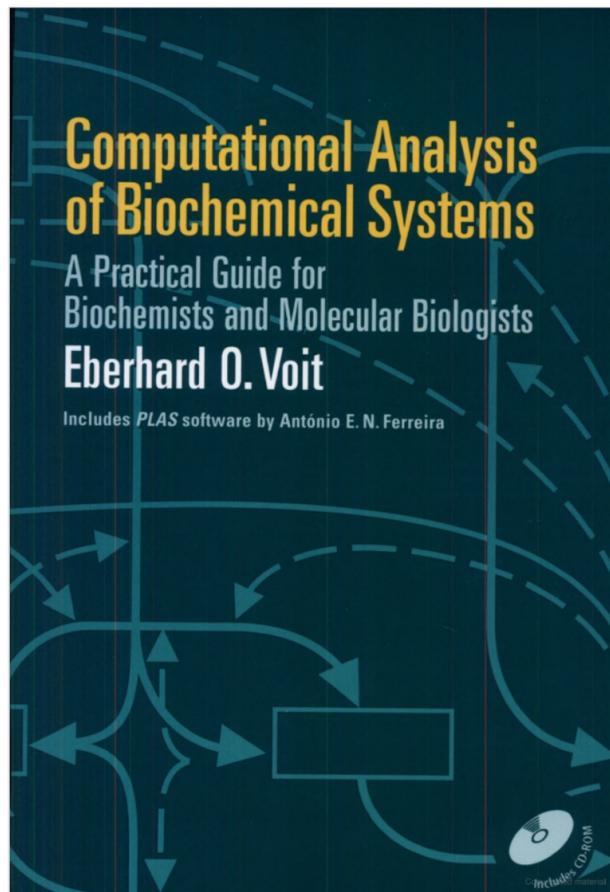




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Metabolic flux and Systems Dynamics
THE ART OF BIOLOGICAL SYSTEMS DYNAMICS SIMULATION AND ANALYSIS

Fluxomics Analysis Report



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Computational Analysis of Biochemical Systems

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FLUXOMICS ANALYSIS REPORT

Fluxomics Analysis Report

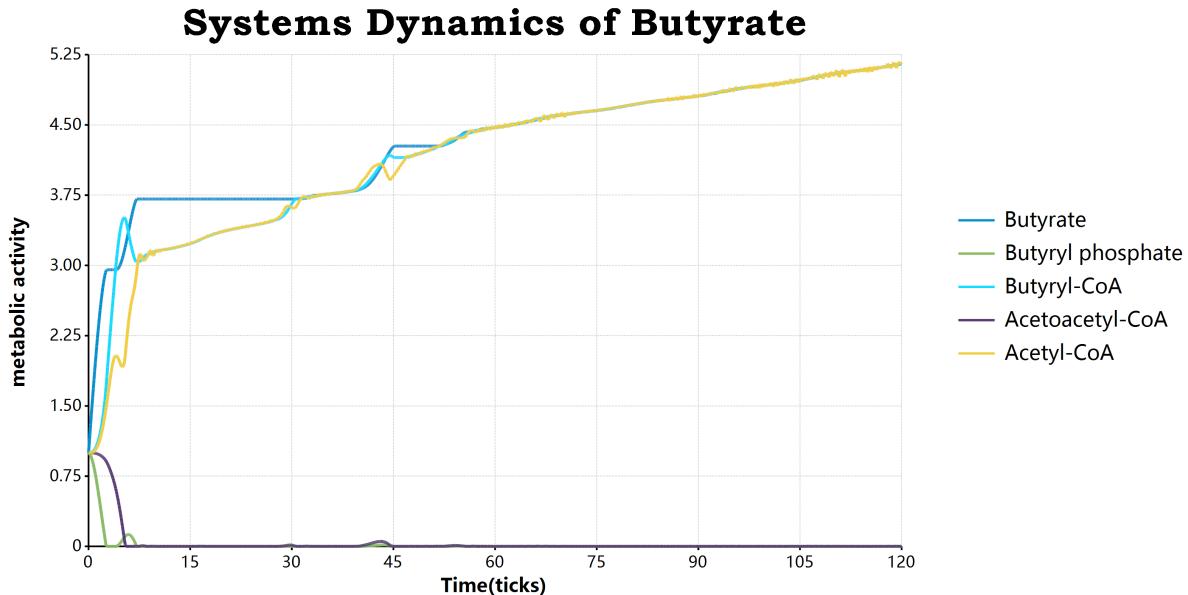
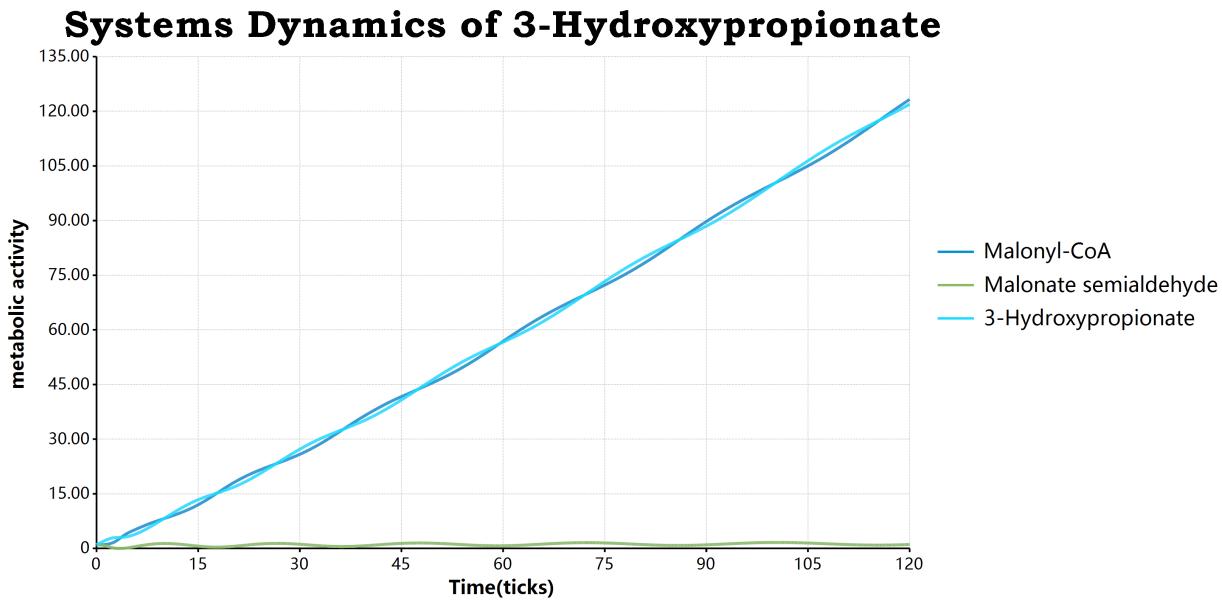
Metabolic flux refers to the amount of a metabolite processed by one or more catalytic steps per unit time, and it is typically normalized by cellular abundance (e.g., gram dry weight) (Stephanopoulos et al., 1998).

A true understanding of genetic and metabolic function and design is facilitated by mathematical and computational methods for analyzing biochemical systems. This hands-on reference teaches biochemists and molecular biologists the use of modern computational methods for the analysis of complex biomedical systems requiring a modest mathematical background. The book begins with representations of biochemical systems, provides guidelines for setting up models, details mathematical and computational methods of parameter estimation and model analysis, and connects to the modern literature with four detailed case studies. Every step is illustrated with examples and explored with accompanying PLAS software. The volume also features over 250 exercises with about one quarter fully or partially solved.

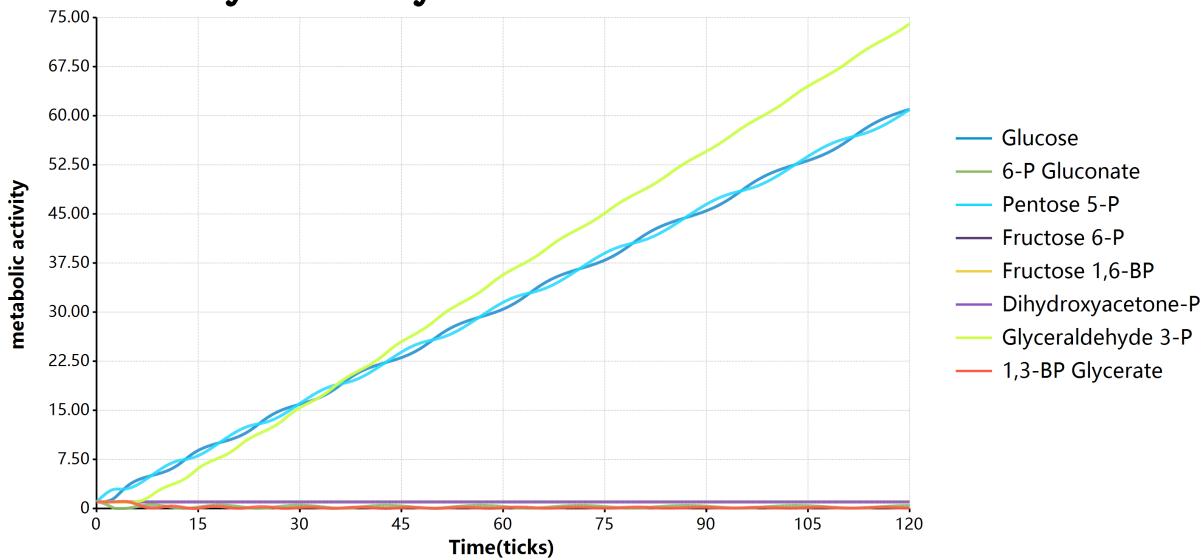
Graph View

Pathway Dynamics

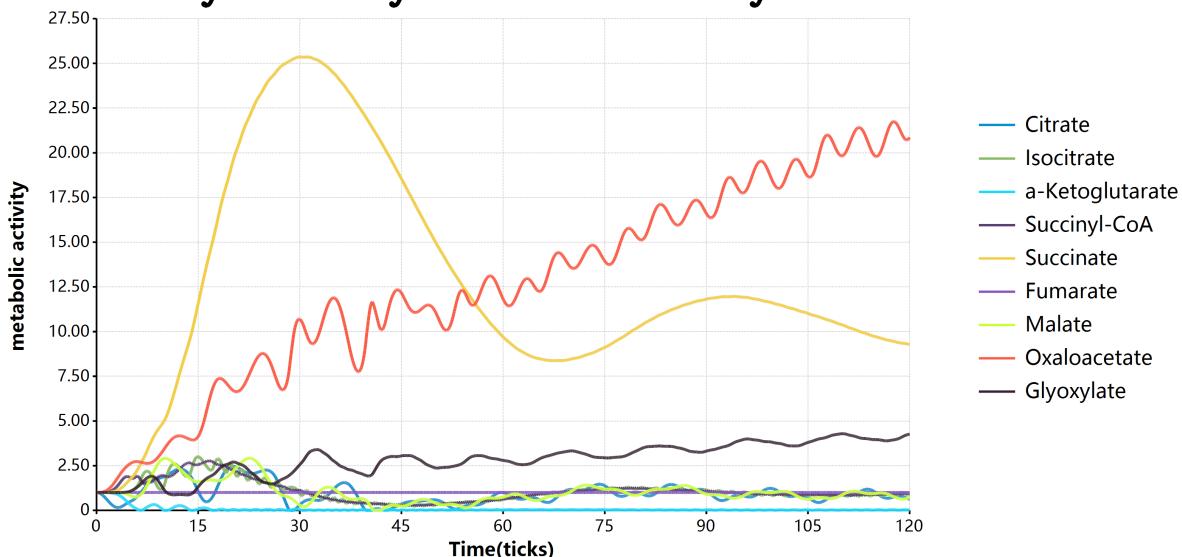
All metabolic changes take place in multiple reactions and follow a particular pathway called the metabolic pathway. The metabolic pathway includes a series of reactions. The metabolite flow, the rate, and direction at which metabolism takes place are called the dynamic state of body constituents.



Systems Dynamics of Pentose



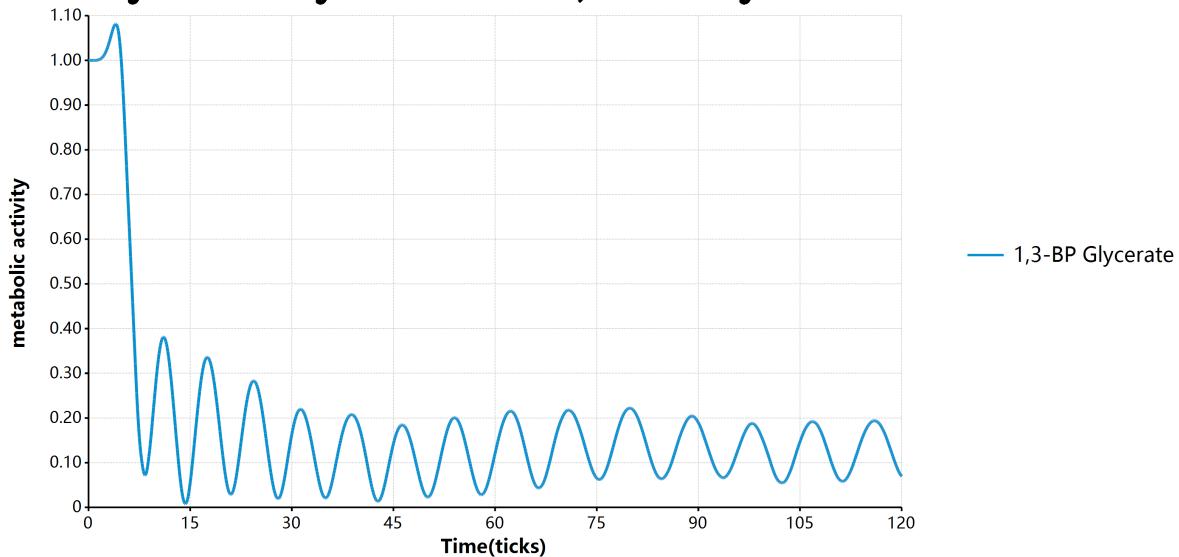
Systems Dynamics of TCA Cycle



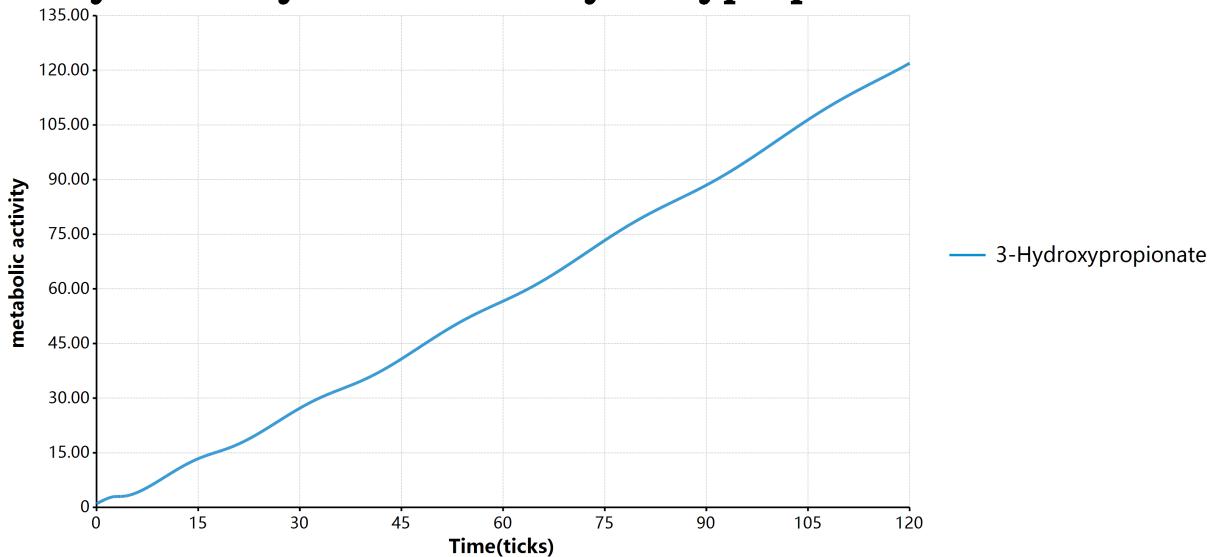
Fluxomics Dynamics

Metabolic flux analysis (MFA) is an increasingly important tool to study metabolism quantitatively. Unlike the concentrations of metabolites, the fluxes, which are the rates at which intracellular metabolites interconvert, are not directly measurable. MFA uses stable isotope labeled tracers to reveal information related to the fluxes. The conceptual idea of MFA is that in tracer experiments the isotope labeling patterns of intracellular metabolites are determined by the fluxes, therefore by measuring the labeling patterns we can infer the fluxes in the network.

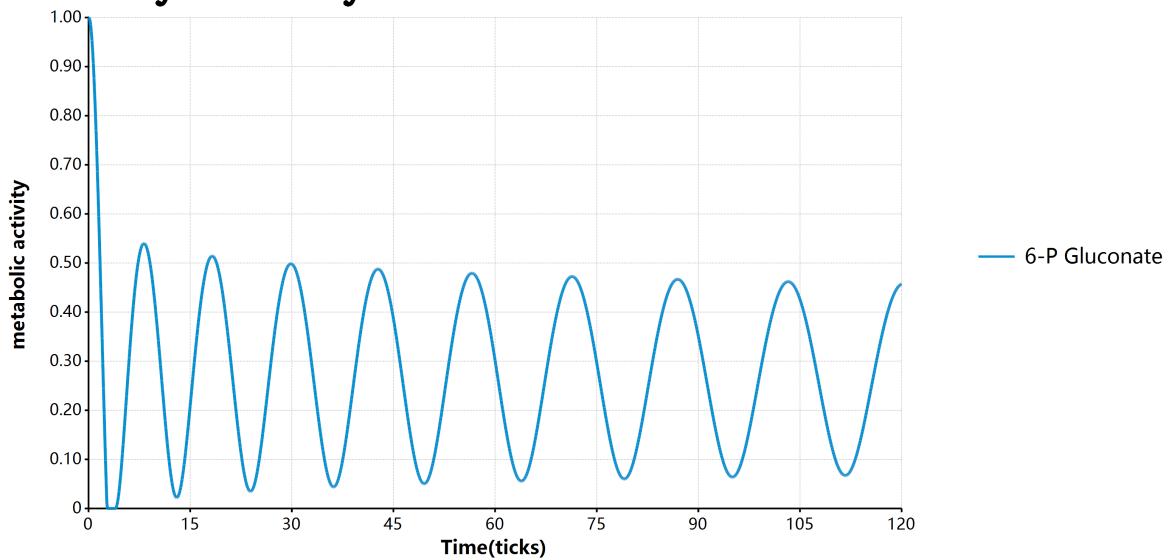
Systems Dynamics of 1,3-BP Glycerate



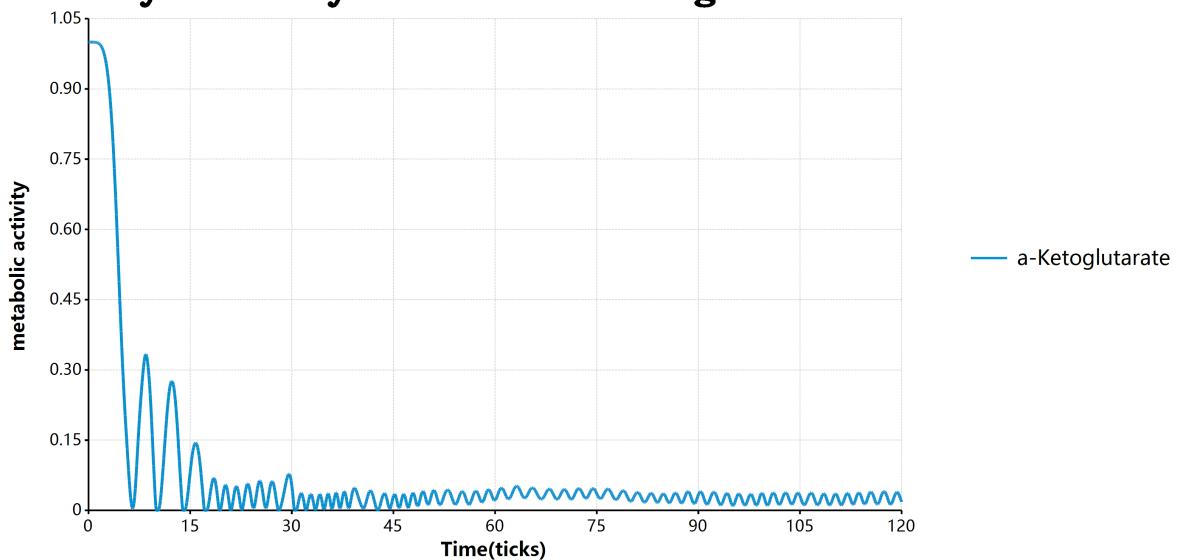
Systems Dynamics of 3-Hydroxypropionate



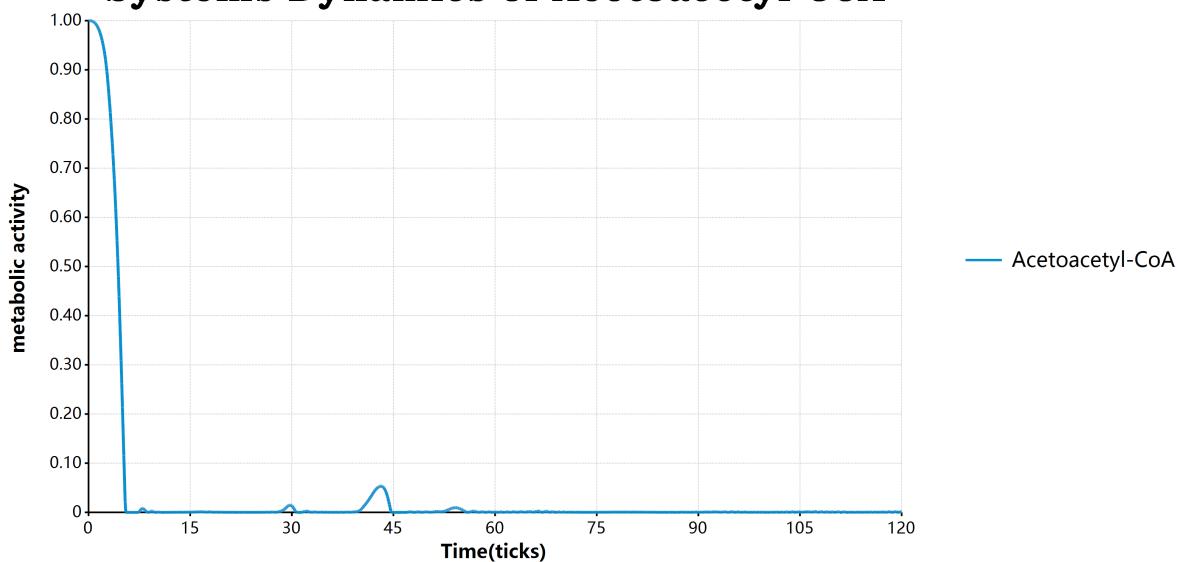
Systems Dynamics of 6-P Gluconate



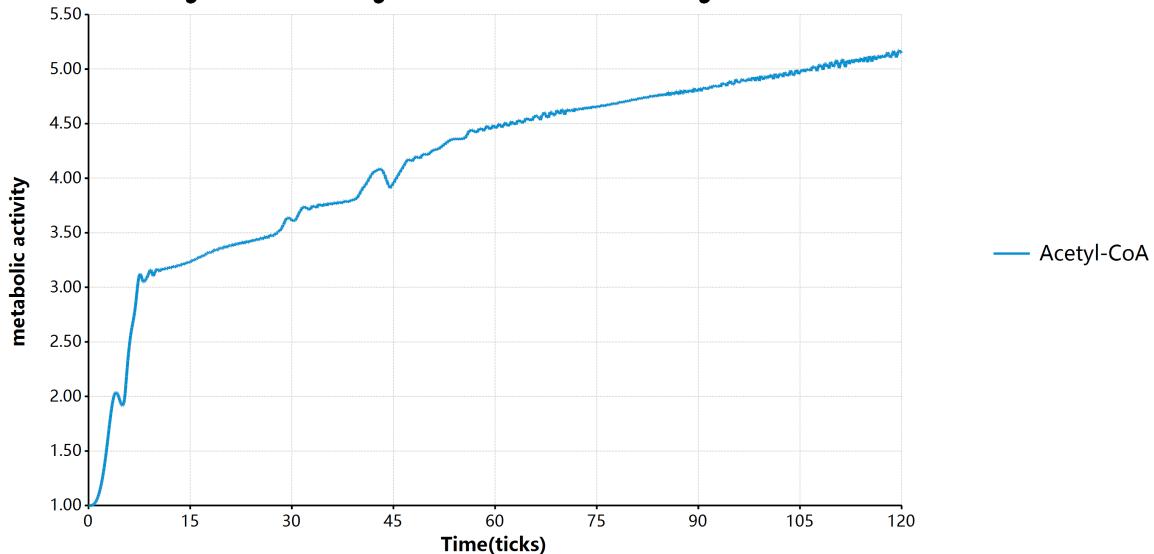
Systems Dynamics of α -Ketoglutarate



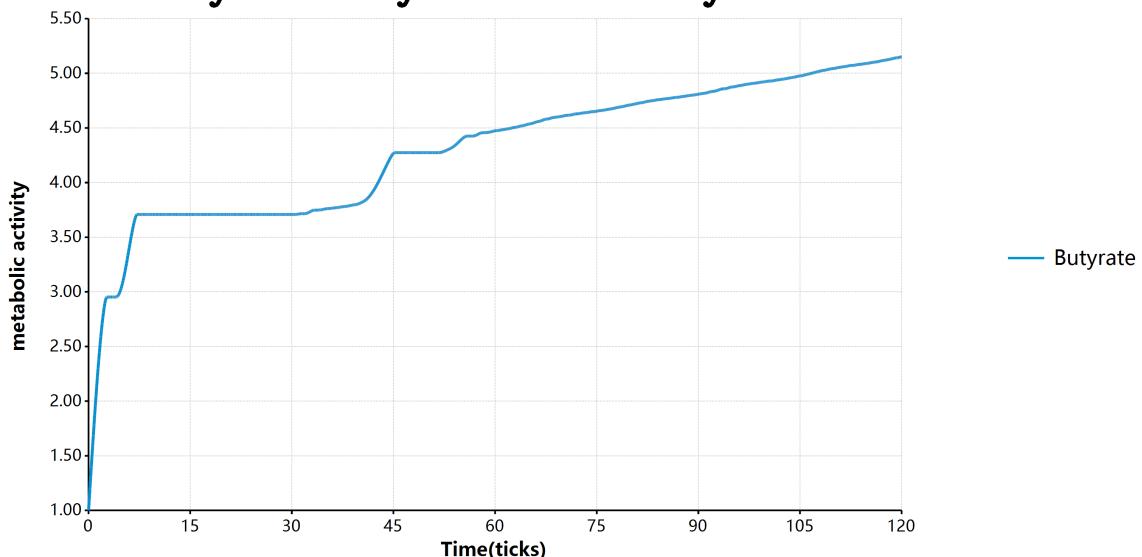
Systems Dynamics of Acetoacetyl-CoA



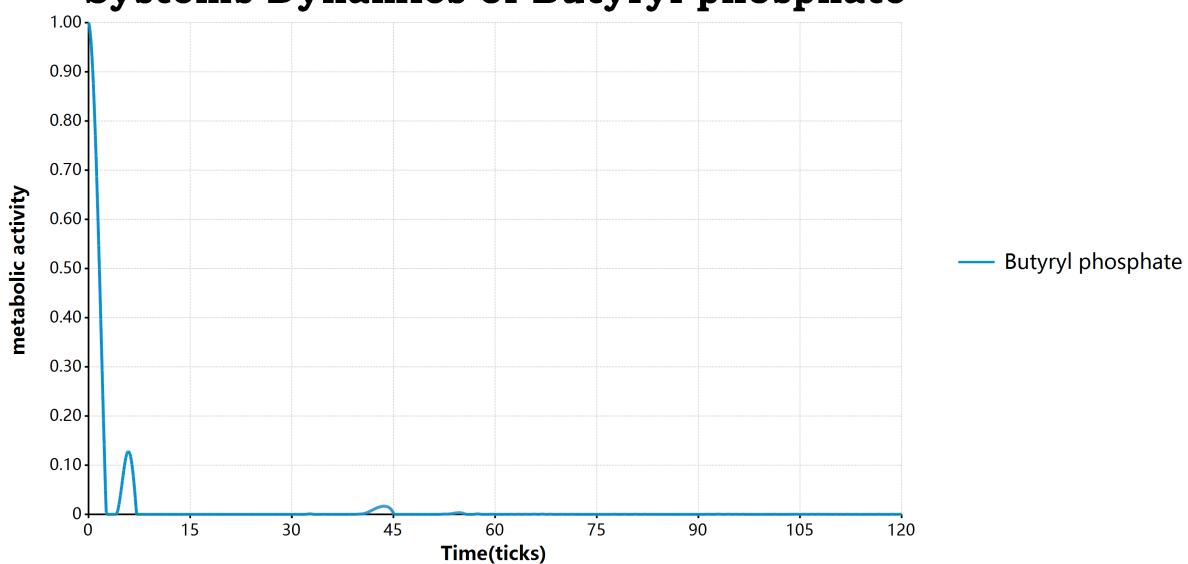
Systems Dynamics of Acetyl-CoA



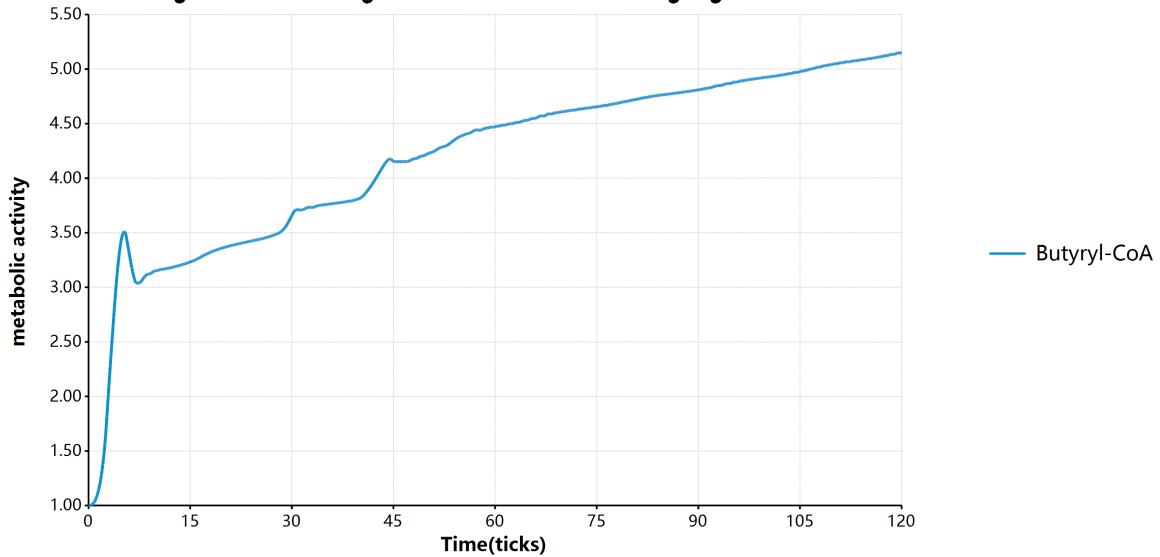
Systems Dynamics of Butyrate



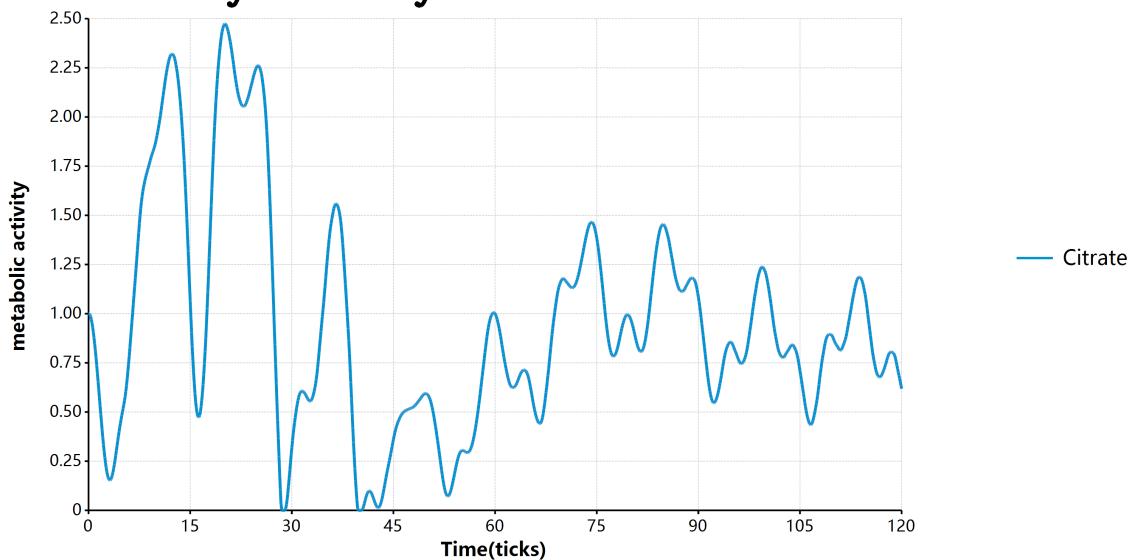
Systems Dynamics of Butyryl phosphate



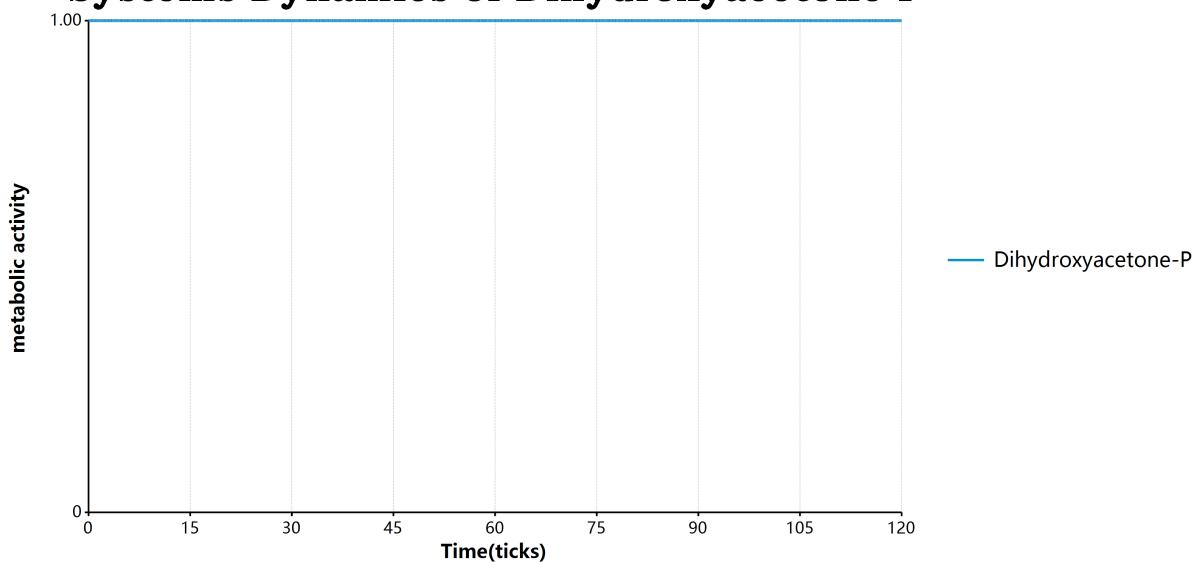
Systems Dynamics of Butyryl-CoA



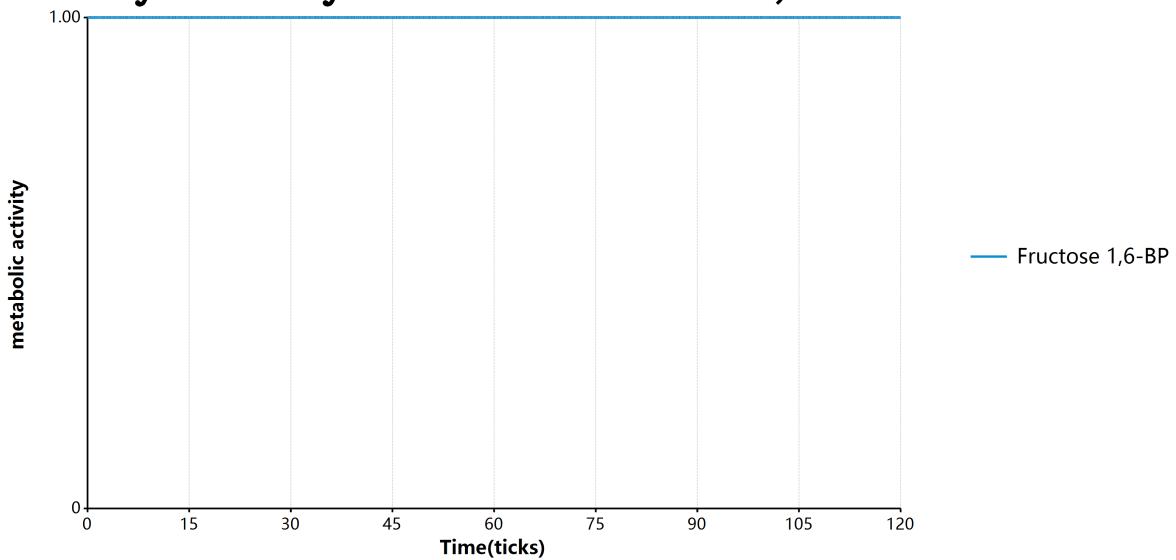
Systems Dynamics of Citrate



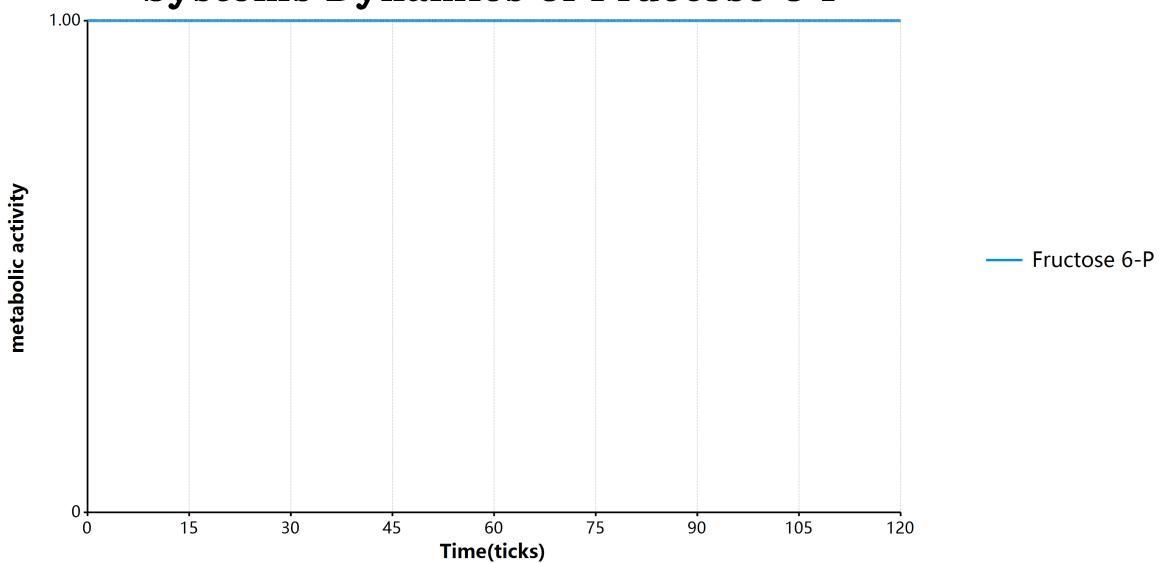
Systems Dynamics of Dihydroxyacetone-P



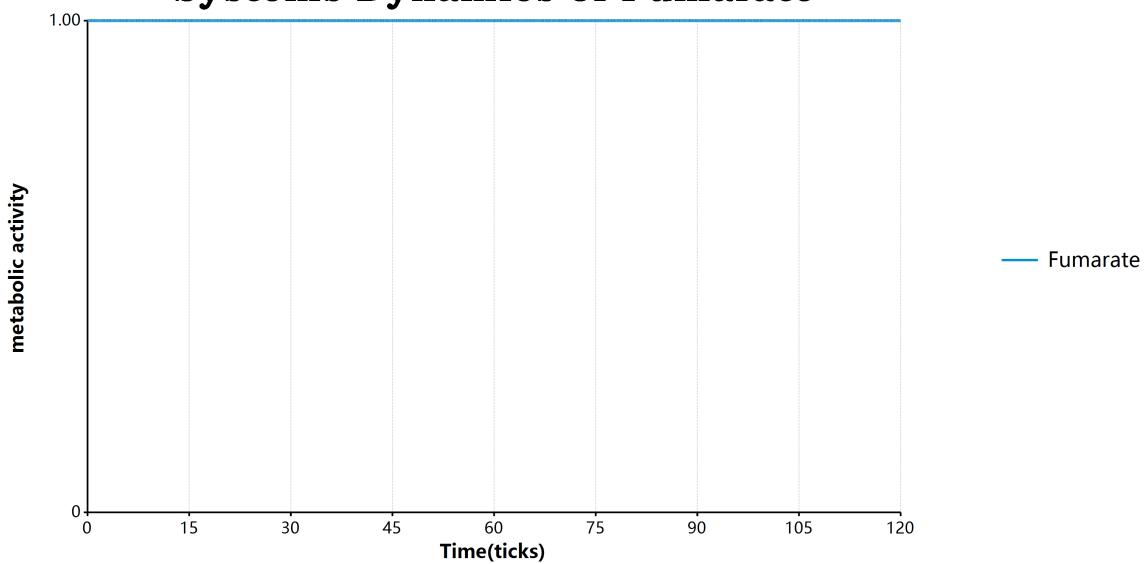
Systems Dynamics of Fructose 1,6-BP



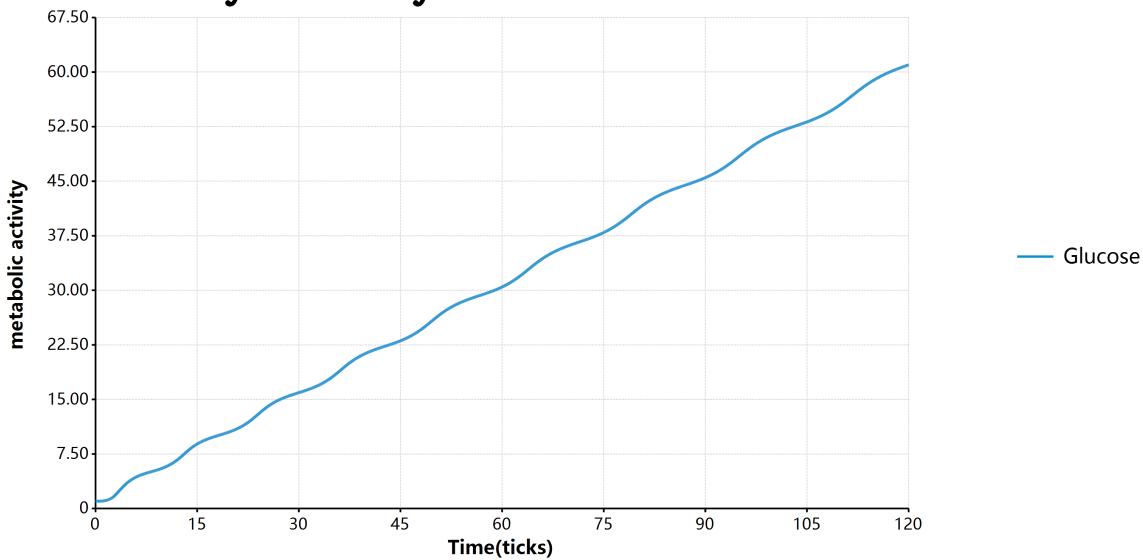
Systems Dynamics of Fructose 6-P



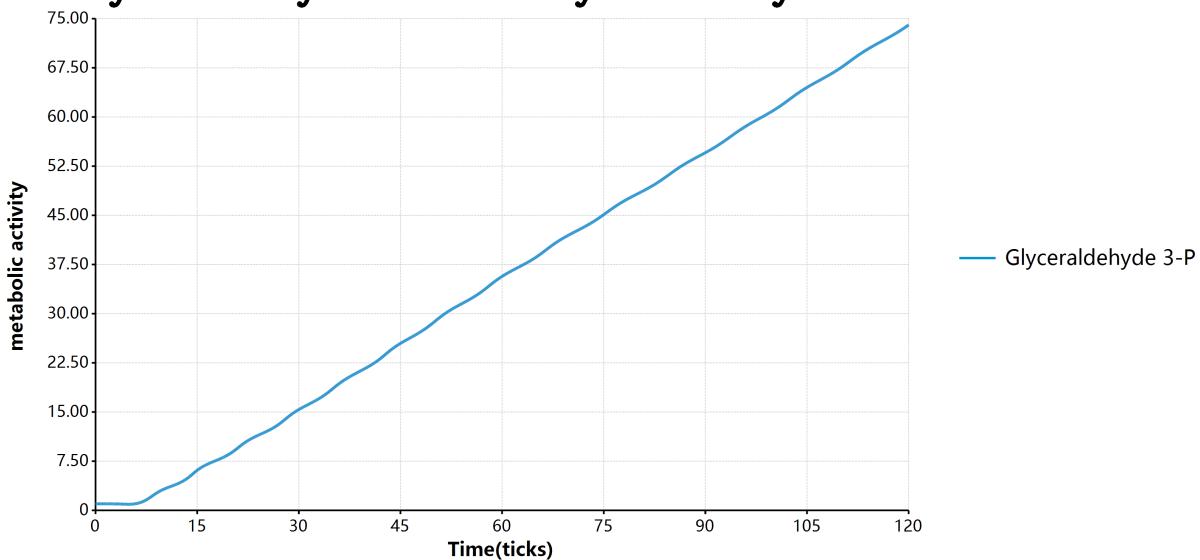
Systems Dynamics of Fumarate



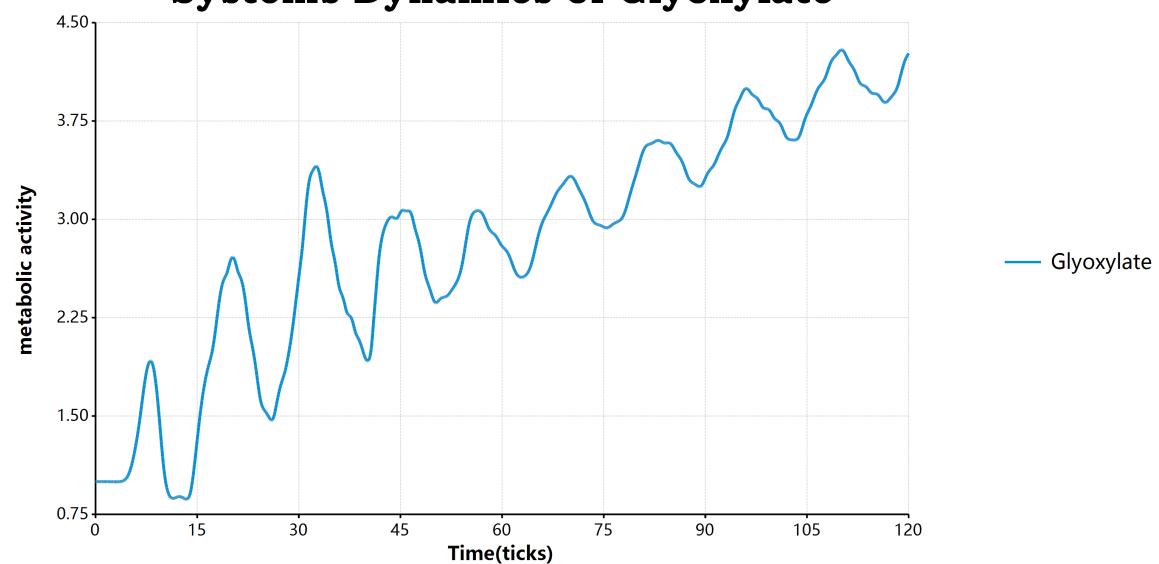
Systems Dynamics of Glucose



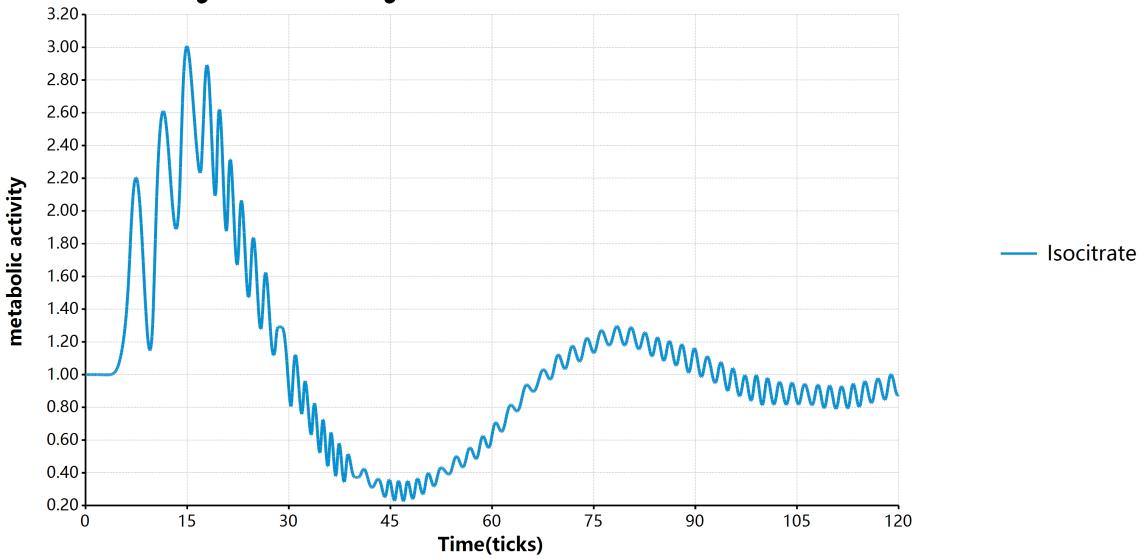
Systems Dynamics of Glyceraldehyde 3-P



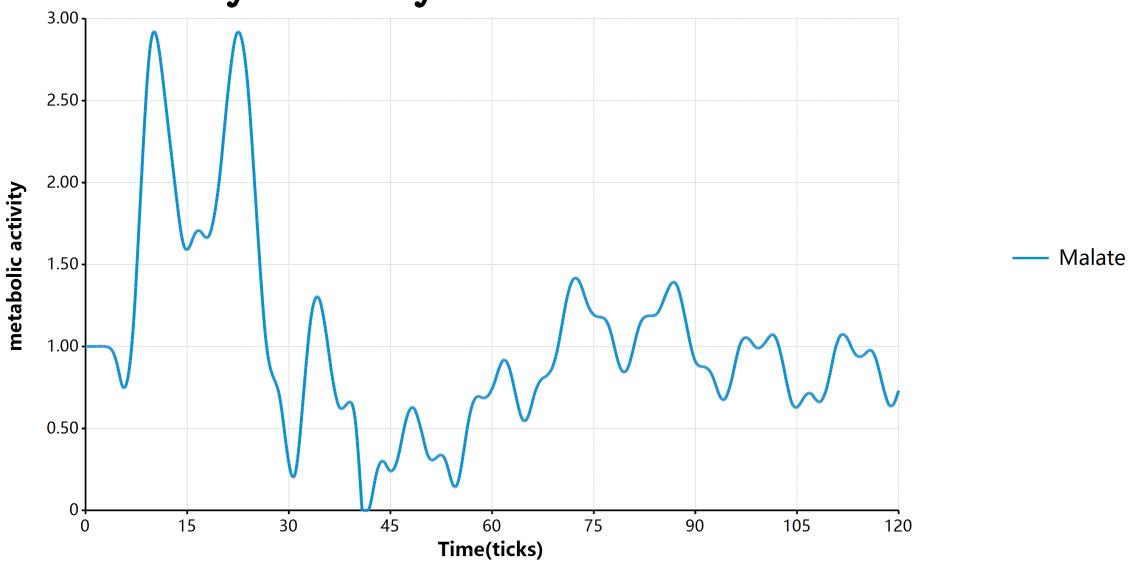
Systems Dynamics of Glyoxylate



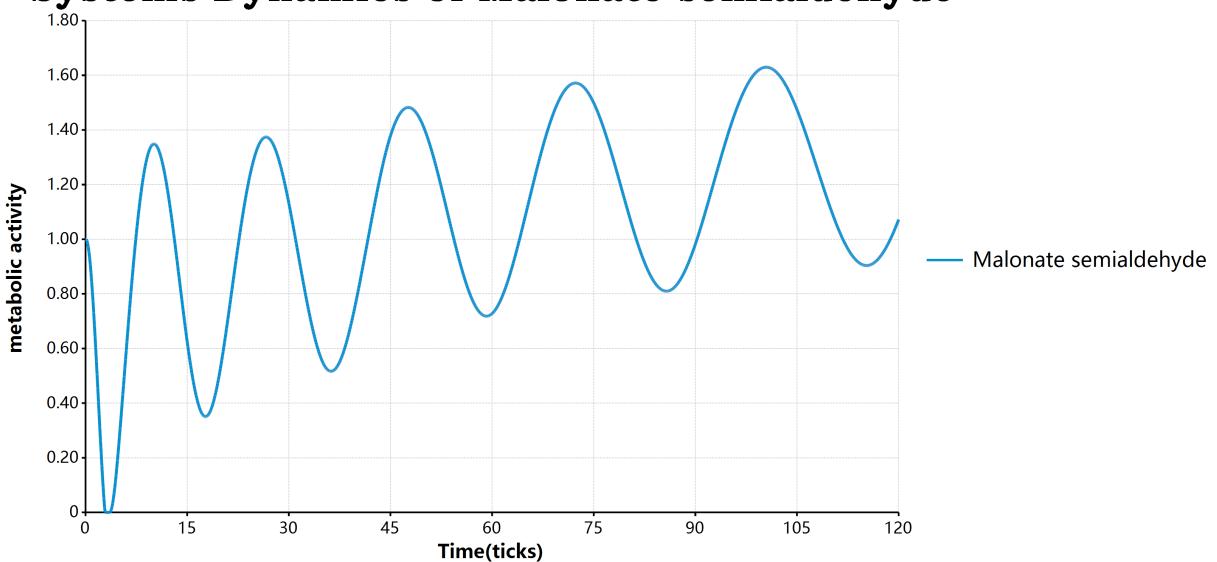
Systems Dynamics of Isocitrate



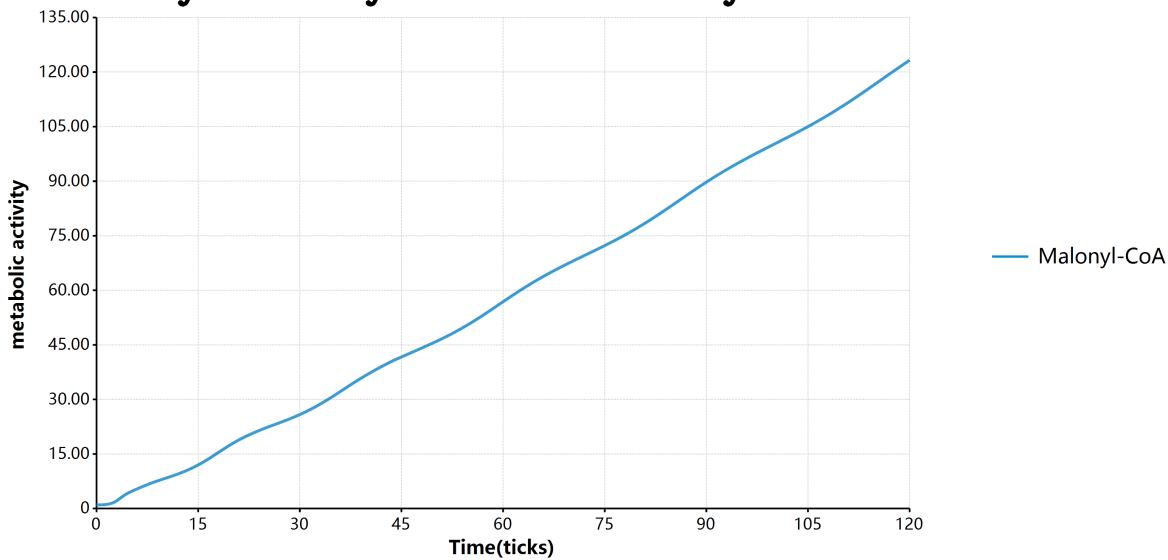
Systems Dynamics of Malate



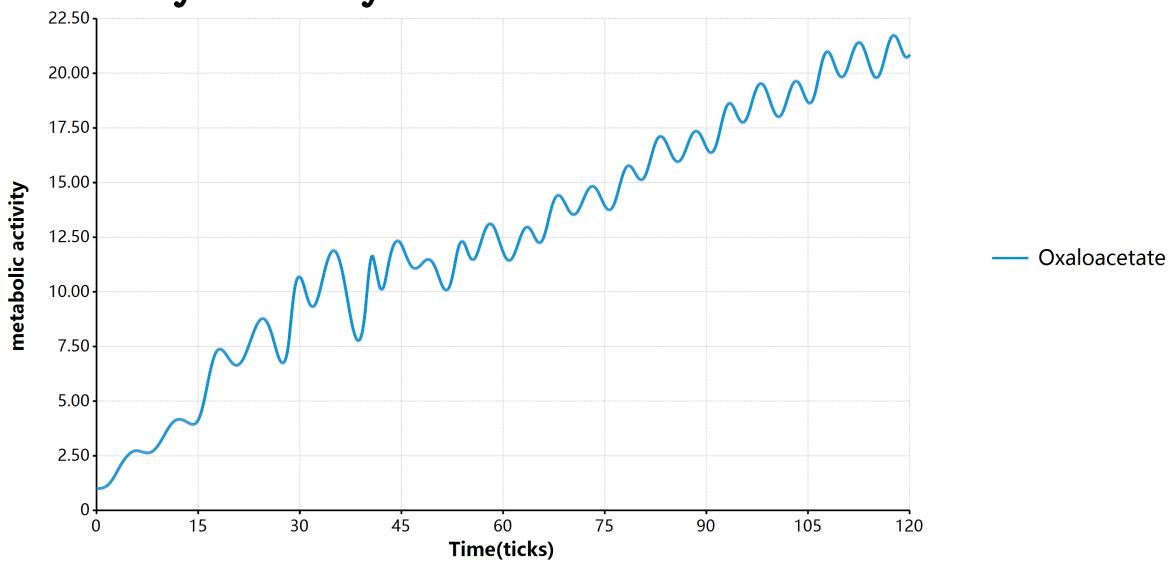
Systems Dynamics of Malonate semialdehyde



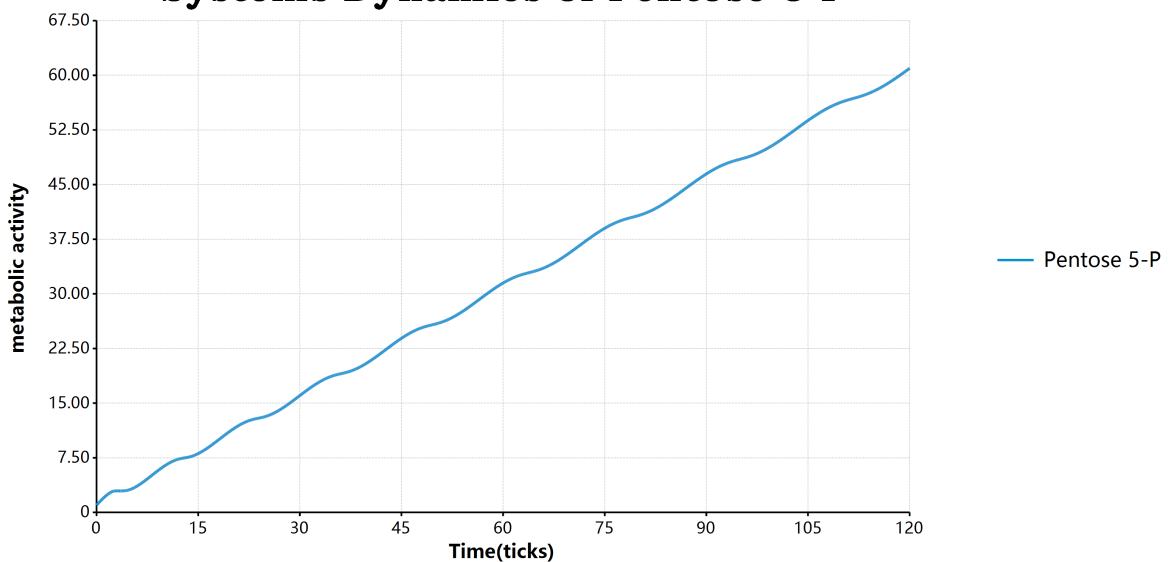
Systems Dynamics of Malonyl-CoA



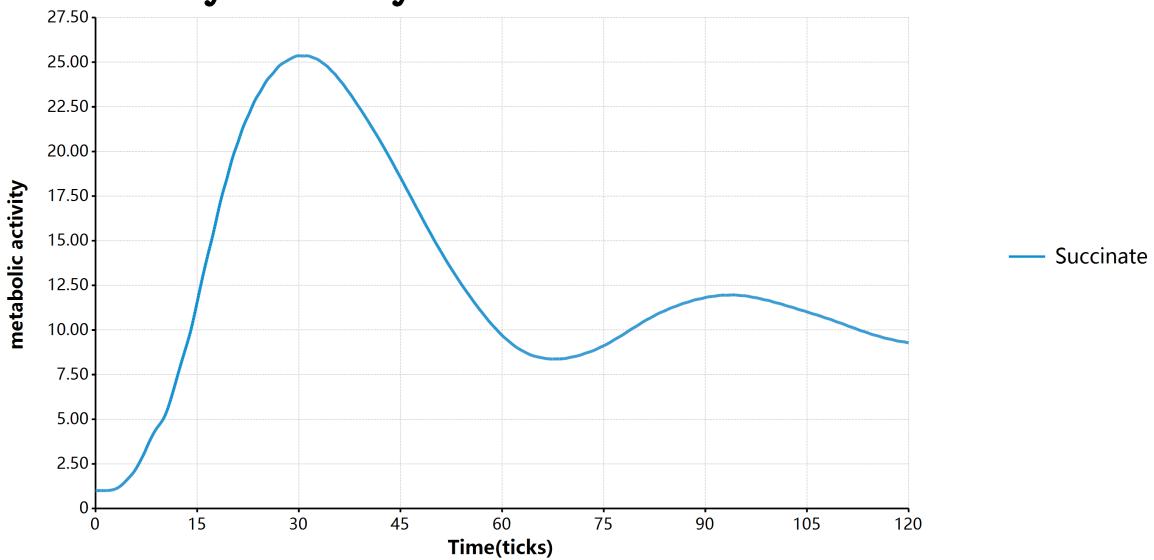
Systems Dynamics of Oxaloacetate



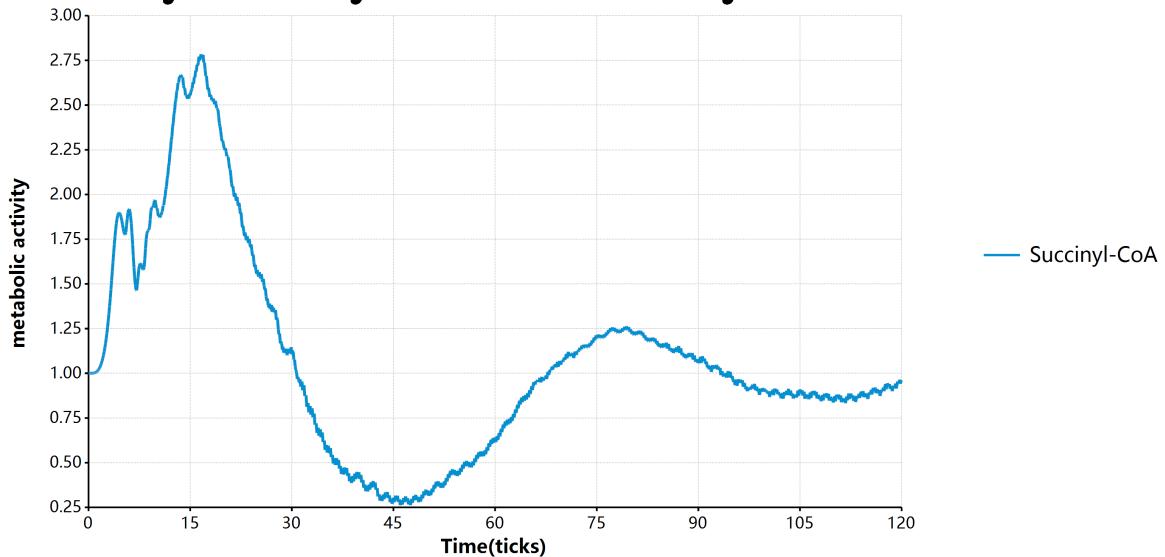
Systems Dynamics of Pentose 5-P



Systems Dynamics of Succinate



Systems Dynamics of Succinyl-CoA



References

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- The Virtual Cell. In Biocomputing: Proceedings of the 1999 Pacific Symposium. R. B. Altman, A. K. Dunker, L. Hunter, T. E. Klein and K. Lauderdale, editors. World Scientific, Singapore. (1999) 228-239. Schaff, J., and L. M. Loew.
- Blinov ML, Schaff JC, Vasilescu D, Moraru II, Bloom JE, Loew LM. Compartmental and Spatial Rule-Based Modeling with Virtual Cell. *Biophys J*. 2017 Oct 3;113(7):1365-1372. doi: 10.1016/j.bpj.2017.08.022. PMID: 28978431; PMCID: PMC5627391.