

The Travel of a Metabolite

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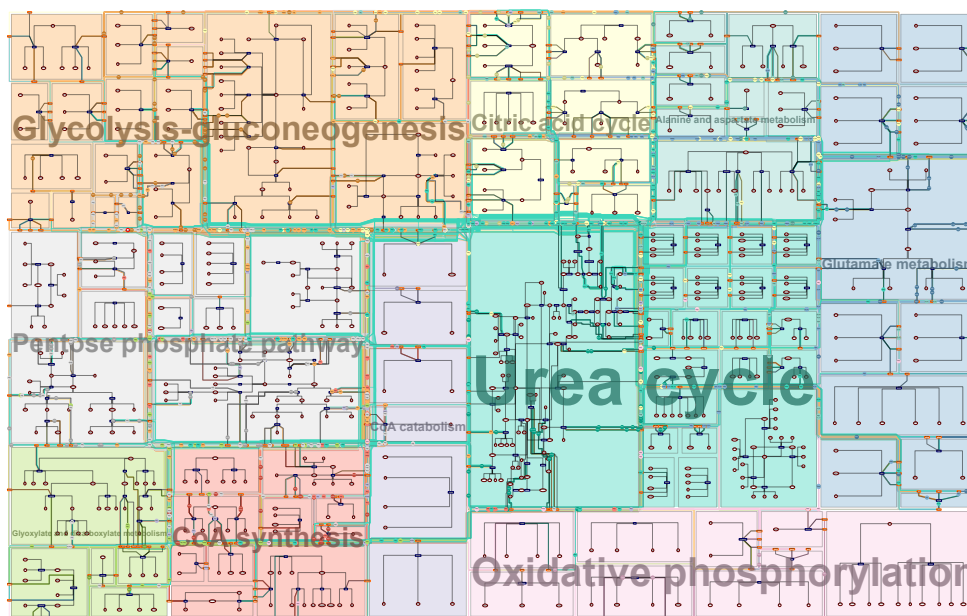


Figure 1: The map of our visual story.

ABSTRACT

Biological pathways are chains of molecule interactions and reactions in biological systems that jointly form complex, hierarchical networks. Although several pathway layout algorithms have been investigated, biologists still prefer to use hand-drawn ones, due to their high visual quality relied on domain knowledge. In this project, we propose a visualization for computing metabolic pathway maps that restrict the grouping structure defined by biologists to rectangles and apply orthogonal-style edge routing to simplify edge orientation. This idea is inspired by concepts from urban planning, where we consider reactions as city blocks and built up roads to connect identical metabolites occurred in multiple categories. We provide a story to present how glucose is broken down to phosphoenolpyruvate to release energy, which is often stored in adenosine triphosphate (ATP) in a human body. Finally, we demonstrate ATP is also utilized to synthesize urea to eliminate the toxic ammonia in our body.

Index Terms: Human-centered computing—Visualization—Visualization techniques—Graph drawings;

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REFERENCES

- [1] Boost C++ Libraries. <http://www.boost.org/>. Accessed: 2018-02-15.
- [2] Human Metabolism. <http://http://www.graphdrawing.de/contest2017/contest.html>. Accessed: 2017-08-15.
- [3] IBM ILOG CPLEX Optimization Studio. <https://www.ibm.com/analytics/data-science/prescriptive-analytics/cplex-optimizer>. Accessed: 2018-02-15.
- [4] Qt 5.8: Cross-platform software development for embedded & desktop. <https://www.qt.io/>. Accessed: 2018-02-15.
- [5] TinyXml. <http://www.grinninglizard.com/tinyxml/>. Accessed: 2018-02-15.
- [6] S. Kieffer, T. Dwyer, K. Marriott, and M. Wybrow. Hola: Human-like orthogonal network layout. *IEEE Transactions on Visualization and Computer Graphics*, 22(1):349–358, 2016.
- [7] A. Noronha, A. D. Danóelsdóttir, P. Gawron, F. Jóhannsson, S. Jónsdóttir, S. Jarlsson, J. P. Gunnarsson, S. Brynjólfsson, R. Schneider, I. Thiele, and R. M. T. Fleming. ReconMap: an interactive visualization of human metabolism. *Bioinformatics*, 33(4):605–607, 2017.
- [8] S. Sutanthavibul, E. Shragowitz, and J. B. Rosen. An analytical approach to floorplan design and optimization. In *Proceedings of the 27th ACM/IEEE Design Automation Conference*, pp. 187–192, 1990.

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