

# Care-free Metabolic Map Editor

— From Pathways to Maps —

Masanori Arita<sup>123</sup>  
arita@k.u-tokyo.ac.jp

- <sup>1</sup> Department of Computational Biology, Graduate School of Frontier Sciences, University of Tokyo and PRESTO JST, Kashiwanoha 5-1-5 CB05, Kashiwa 277-8561, Japan
- <sup>2</sup> Institute of Advanced Biosciences, Keio University, Tsuruoka-shi Baba-cho 14-1, Yamagata 997-0035, Japan
- <sup>3</sup> Computational Biology Research Center, Koto-ku Aomi 2-43-17, Tokyo 135-0064, Japan

**Keywords:** metabolism, network, tracer experiments

## 1 Introduction

For most biochemists, drawing metabolic maps for a research paper or a web page means too much labor and trouble; an exact copy of existing maps may infringe their copyrights whereas laying out from scratch requires detailed knowledge on metabolism, such as substrate specificity or chirality.

Why isn't there any software tool that can depict, or at least modify, ready-made metabolic maps by mouse clicks? Its reason is rooted in the current knowledge representation of metabolic databases, where structural information of metabolites is completely ignored despite the fact that **the substrate-product structure relationship is indispensable information in reliable pathway reconstruction**. To verify this observation, we designed the Atomic Reconstruction of Metabolism (ARM) software that can computationally reproduce biochemical radioisotope-tracer experiments (Figure 1; see also [1, 2]). This year's presentation introduces its extension, i.e. 'care-free metabolic map editor' that can compile and edit metabolic pathways into maps.

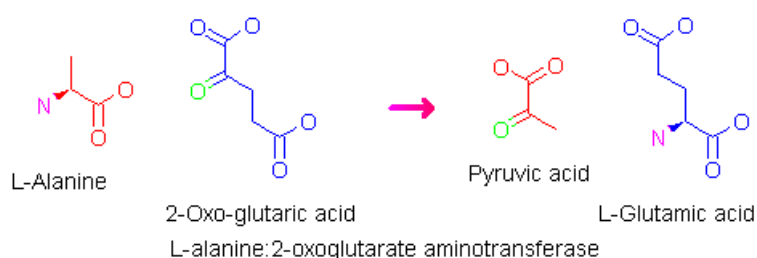


Figure 1: EC 2.6.1.2 aminotransferase

An example reaction among four metabolites. In the nitrogen metabolism, the reaction is considered a link between L-Alanine and L-Glutamic acid, but in the carbon metabolism, L-Alanine is linked with Pyruvic acid. Since most metabolic reactions involve three or four metabolites, the interpretation of each reaction changes depending on its context.

## 2 Methods and Results

The metabolic map editor provides basic drawing functions like those of PowerPoint (Microsoft, Redmond, WA). The editor is coupled with a search window for metabolic pathways, and searched results

are visualized by drag-and-dropping them on another canvas window. The positioning and drawing of metabolite structures are automatic, and modification of drawn objects is possible as in PowerPoint. Thus, a user can draw and edit metabolic maps of interest basically through mouse operations.

A notable characteristic of this metabolic editor is that **the substrate-product structure relationship is implicitly associated throughout all edit operations.** Therefore, a user can trace any carbon or nitrogen atom on any arbitrarily drawn map. Its tracing result follows the wys-wyg style; all and only drawn enzymatic arrows are traversed according to the drawn directions, and all possible destinations are highlighted. The attachment of comments, quantitative information, and internal and external links is also supported. The software tools and data are freely available at <http://www.metabolome.jp/>.

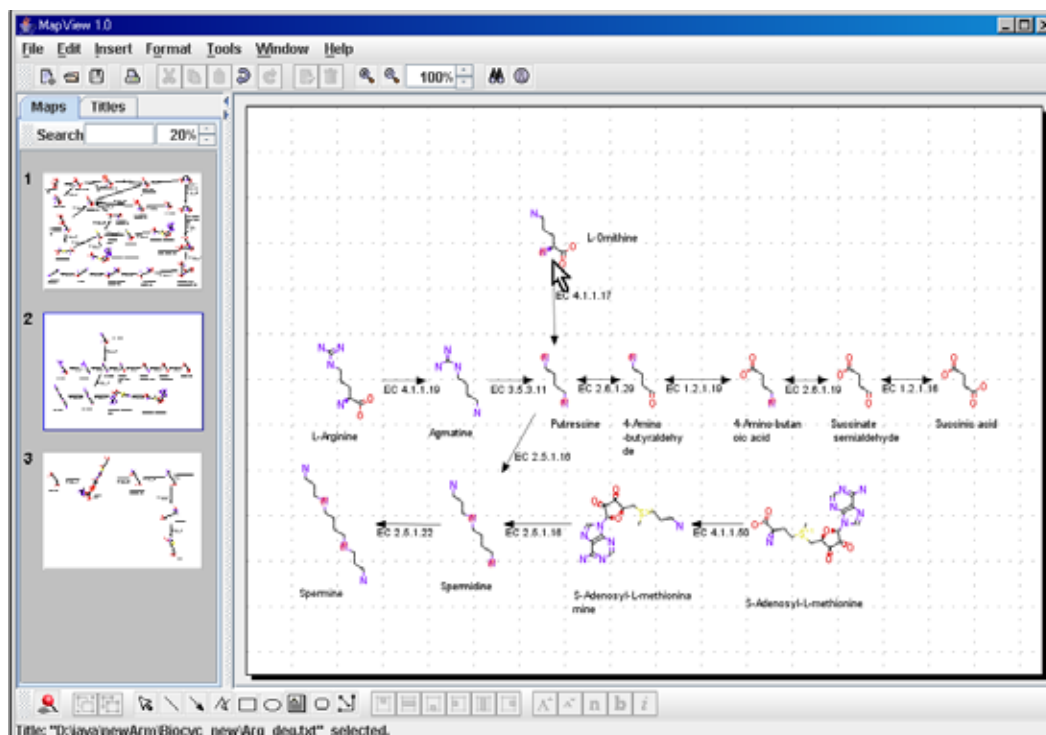


Figure 2: ARM Metabolic Map Editor

## Acknowledgments

This work was initially supported by IPA, Exploratory Software Project, 2003, and subsequently by MEXT, Grant-in-Aid for Scientific Research on Priority Areas, 16014206, 2004.

## References

- [1] Arita, M., In silico atomic tracing by substrate-product relationships in *Escherichia coli* intermediary metabolism, *Genome Res.* 13(11) 2455–2466, 2003.
- [2] Arita, M., The metabolic world of *Escherichia coli* is not small, *Proc. Natl. Acad. Sci. USA* 101(6) 1543–1547, 2004.