

Atomic Reconstruction of Metabolism: Metabolic Map Editor

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- Major application area: Metabolism, Bioprocess, Metabolome analysis
- Platform: Windows, Mac, Linux
- Availability: freely downloadable
- Where or how to obtain the software: <http://www.metabolome.jp/>

It is not straightforward to manually trace metabolic pathways, because molecular structures of substrates are rearranged into products in each reaction step. The recombination of structures must be formally represented, including structural symmetry and chirality, to computationally hypothesize alternative metabolic pathways or to verify capability of biosynthesis or degradation. As an example, it was shown that *E. coli* metabolic network is not a small world if carbon atoms are correctly traced in the network [1]. Atomic Reconstruction of Metabolism (ARM) is a software program designed to explore and visualize logical traces of arbitrary metabolic pathways in a defined network. Each reaction step is decomposed into a set of “substructural correspondences” between metabolites [2], and any pathway can be searched by combining these correspondences. The search results can be drag-and-dropped on the main window, where a user can merge and arrange pathways to construct a metabolic map as in a conventional drawing editor. It is also possible to superimpose gene expressions and metabolite concentrations on the user-defined map. The flexibility to rearrange and design metabolic maps drastically accelerates all types of metabolic analysis. Users can design a metabolic map for each sequenced species, and grasp its metabolic capability without referencing shredded pieces of metabolic pathways in books or traditional databases. Another advantage is that it can substitute abstract description with concretes such as assigning particular fatty acids for phosphatidyl moieties. It is one of the pioneering software to analyze fatty acid metabolism and metabolism for other polymeric moieties.

References

[1] Arita, M. "The metabolic world of *Escherichia coli* is not small."

Proceedings of the National Academy of Sciences USA, 101(6) 1543-1547, 2004.

[2] Arita, M. "*In silico* Atomic tracing by substrate-product relationships in *Escherichia coli* intermediary metabolism." *Genome Research*, 13(11) 2455-2466, 2003.