

Mining the KEGG pathway database with self-organizing maps

Egon Willighagen 

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Abstract

The Self-organizing map (SOM) is a popular (again) and intuitive non-linear mapping method: it transforms a multidimensional space into two dimensions (normally: they are so easy to visualize). Latino and Aires-de-Sousa published a paper that uses this method to analyze the whole KEGG pathway database: Genome-Scale Classification of Metabolic Reactions: A Chemoinformatics Approach (DOI: [anie.200503833](https://doi.org/10.26434/chemrxiv-2005-anie)).

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The [Self-organizing map](#) (SOM) is a popular (again) and intuitive non-linear mapping method: it transforms a multidimensional space into two dimensions (normally: they are so easy to visualize). Latino and [Aires-de-Sousa](#) published a paper that uses this method to analyze the whole [KEGG pathway database](#): *Genome-Scale Classification of Metabolic Reactions: A Chemoinformatics Approach* (DOI: [anie.200503833](#)).

The method is based on earlier work by Zhang and Aires-de-Sousa: *Structure-Based Classification of Chemical Reactions without Assignment of Reaction Centers* (DOI: [10.1021/ci0502707](#)). A non-trivial feature of the suggested method is the use of two SOMs. The first maps the reaction onto a fixed-length vector (coined MOLMAP), which is used as input vector for the second map. This later map is used to cluster the KEGG reactions on a purely chemical basis. The resemblance with the [EC numbering system](#) is striking.