

Genome-scale classification of metabolic reactions: a Chemoinformatics approach

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Classification of enzymatic reactions plays a central role in the reconstruction of metabolic pathways, prediction of metabolism, or development of biotechnological processes.

We have developed a method for reaction representation that avoids identification of the bonds and atoms involved in the reaction (reaction center), is based on local physicochemical parameters, and consists of a fixed-length numerical code – MOLMAP descriptor (*Angew. Chem. Int. Ed.* **2006**, *45*, 2066-2069).

Here we show the mapping of a genome-scale set of 3468 enzymatic reactions by a self-organizing map (or Kohonen neural network) on the basis of the MOLMAP reaction descriptor. The approach shows a general compatibility with the well-established EC numbers, and overcomes some of their limitations for diversity analysis of the reactome. Examples are presented that show how a map of enzymatic reactions can reveal similarities between reactions with strong differences in EC numbers, and identify misclassifications in reaction databases.