

Automated metabolic pathway reconstruction based on structural grammars

Rajat K De¹ and Somnath Tagore²

¹Indian Statistical Institute, India

²Dr. D. Y. Patil University, India

Analyzing is extremely essential, which can be used for predicting outcomes of different metabolic pathways as well as studying their metabolic dynamics. Till date, various strategies have been proposed for modeling a metabolic pathway. However, the method for reconstruction of a metabolic pathway from a given set of biochemical reactions is not easily available.

Here we describe a novel algorithm that we have recently developed for automated metabolic pathway reconstruction and modeling. The algorithm generates a metabolic pathway using some given structural representations of metabolites, which in this case is SMILES (Simplified Molecular Input Line Entry System). Using this algorithm, any metabolic pathway can be reconstructed, based on some thermodynamic thresholds and structural properties. The effectiveness of the algorithm is demonstrated on pathway datasets of 25 and 24 metabolic pathways of *Mycoplasma pneumoniae* M129 and *Homo sapiens* respectively. The dataset is taken from KEGG and PubChem Compound data repositories.

The results show pathway reconstruction average accuracy of 91% in *M. pneumoniae* M129 and 96% in *H. sapiens*. The algorithm is also able to detect multiple reaction links for a metabolite, based upon a pre-assigned threshold value. Furthermore, the connectivity prediction average accuracy of the algorithm has been found to be 97% in *M. pneumoniae* M129 and 96% in *H. sapiens*. Overall, the algorithm performs better than some others including Copasi, PHT, Gepasi, Jarnac and Path-A.

Biography

Rajat K. De is an Associate Professor of the Indian Statistical Institute, Kolkata, India. He obtained his Ph.D. degree from the Indian Statistical Institute, India, in 2000. Rajat De was a Distinguished Postdoctoral Fellow at the Whitaker Biomedical Engineering Institute, the Johns Hopkins University, USA, during 2002-2003. He has published about 30 research articles in International Journals. His research interest includes bioinformatics, computational biology, systems biology, pattern recognition and soft computing.

rajat@isical.ac.in