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Automated metabolic pathway reconstruction based on structural grammars

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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

Dr. 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. Dr. 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.