In silico knock out screening of the metabolic network of *plasmodium falciparum* to yield Potential Drug Targets

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1.0 Introduction

We developed a simple tool which analyzes metabolic pathways and identifies essential reactions/enzymes that may be considered as drug targets. Our approach limits time and cost consuming wet experiments.

2.0 Materials and Methods

The metabolic network of *plasmodium falciparum* was constructed with 554 metabolites and 575 metabolic reactions [1], each compound can be substrate and product. The metabolites and reactions are considered as node and edges respectively

Our greedy algorithm investigates the essentiality of a reaction when it is knocked out on the metabolic network. Following a strategy put up recently [2] the algorithm works as follows:

1. *Verify the essentiality of a deleted reaction.*
2. *Create the variety of products.*
3. *Minimize the number of reactants and reactions to produce the products*
4. *Compare the results of wild-type and mutated network*

3.0 Results and Discussion

203 reactions were identified as essential in the network. About 40% of the essential reactions are in the list of choke points found elsewhere [3]. Also 25% about were highly expressed when analyzed [Genesis] and clustered into 6 groups. We are presently validating our possible targets with wet laboratory experiments.

4.0 Conclusion

Our approach is not computationally expensive and not time consuming even though we are applied a greedy algorithm approach. Additionally to other approaches, we carefully check for alternative pathways generating products of choke points [3]

References

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