Predicting new drug indications from network analysis

Yousoff Efendy Mohd Ali*, Kiam Heong Kwa† and
Kurunathan Ratanavelu‡

Institute of Mathematical Sciences
Faculty of Science, University of Malaya
Kuala Lumpur 50603, Malaysia

*yousoff92@gmail.com
‡kkwa@um.edu.my
§karun052001@gmail.com

Received 6 July 2017
Accepted 16 September 2017
Published 4 October 2017

This work adapts centrality measures commonly used in social network analysis to identify drugs with better positions in drug-side effect network and drug–indication network for the purpose of drug repositioning. Our basic hypothesis is that drugs having similar phenotypic profiles such as side effects may also share similar therapeutic properties based on related mechanism of action and vice versa. The networks were constructed from Side Effect Resource (SIDER) 4.1 which contains 1430 unique drugs with side effects and 1437 unique drugs with indications. Within the giant components of these networks, drugs were ranked based on their centrality scores whereby 18 prominent drugs from the drug-side effect network and 15 prominent drugs from the drug–indication network were identified. Indications and side effects of prominent drugs were deduced from the profiles of their neighbors in the networks and compared to existing clinical studies while an optimum threshold of similarity among drugs was sought for. The threshold can then be utilized for predicting indications and side effects of all drugs. Similarities of drugs were measured by the extent to which they share phenotypic profiles and neighbors. To improve the likelihood of accurate predictions, only profiles such as side effects of common or very common frequencies were considered. In summary, our work is an attempt to offer an alternative approach to drug repositioning using centrality measures commonly used for analyzing social networks.

Keywords: Network analysis; drug network; drug development.

PACS Nos.: 89.75.Hc, 89.90.+n, 89.75.–k.

1. Introduction

The development of each new drug may cost a staggering amount of $500 to more than $2000 million and consume between 10 and 15 years. The figures kept on increasing in 2013 with an estimated pre-tax industry cost of $2558 million per drug

†Corresponding author.
31 December 2016.


