CHAPTER 5 CONCLUSIONS AND SUGGESTIONS

5.1 Conclusions

ADRs are currently the major problems that make the attrition in public health and pharmaceutical industry. The understanding of ADRs can be supported by systems pharmacology which studies the effects of medication in the complex network. Moreover, the integrations of different resources and knowledge discovery can expand the intelligence and enhance the functional predictions. Even though there are several benefits to experience this information, no repository has been stored certain data. A prototype database for ADRs has thus been developed in this work to responsible for the point.

Database for ADRs has been constructed from the linkage consequences of three associations: ADR-drug, ADR-protein, and drug-protein. Along these, only ADR-protein associations are the results from literature mining and have to be proved for consistency. The comparative of known studies indicates that the literature mining process can faithfully extract protein to link with ADR. The identical technique is applied to test the linked ADR-drug-protein associations. The findings can also be assumed that database for ADRs is able to generate the appropriate associations between ADR, drug, and protein. Furthermore, the predictive scores of drugs for hepatobiliary disorders are forecasted by K-nearest-neighbor model and can promote the examination about ADRs.

The constructed database for ADRs contains 130,446 ADR-drug-protein associations which 70,579 are ADR in group of hepatobiliary disorders. The database is represented in web browser with an easy-to-use interface. It initially displays the results of question and interesting related entity which can be expanded to observe the remained substance from ADR-drug-protein relationships in table and can be downloaded for details of entities. Additionally, database for ADRs provides the hyperlink to uncover related pathway using functional annotation tool in DAVID and user guide which make comprehensible utilization.

As in demonstrations, database for ADRs has the ability to give the known information and suggest the possible entities which are related to the desirable objects from different users. These are beneficial for making the precaution and further study. In conclusion, database for ADRs is a powerful tool which can be used in the examinations of ADR and relevant entities.

5.2 Suggestions

(1) Because of the restricted access to the full text of papers, the ADR-protein relationships were only extracted from abstract that stored in PubMed using literature mining tool. The full potential of literature mining approach should be able to pull out information from the entire of literary production, including citation information,

figures, and tables. Another difficulty was the lack of standardization of gene or protein names. The development for resolving ambiguity in the names is important to literature mining. Lastly, rather than manual review, the methodical approach to identify the pattern of associations in a semantic manner is also essential to advance literature mining process.

(2) Predictive scores of drug for hepatobiliary disorders were forecasted from nine quantitative structure-properties using K-nearest-neighbor classification model. There were still several characteristics of drug and classification algorithms for predicting the most accurate possibility of drugs to cause hepatobiliary disorders. Furthermore, predictive scores for possible ADR were general forecast on system organ class of hepatobiliary disorders. This could be more beneficial to users, especially doctors and patients, if the predictive scores were determined on each ADR.

(3) In the illustrations of how to examine, database for ADRs can be used to nominate the probable ADR, drug, and protein from questions of different users. This information brings an awareness of ADR which should have the experiments specially designed and performed to confirm and make the conclusion stronger.

(4) In addition to three relationships constructing database for ADRs, there remained interactions that could be introduced in this systems approach. Drug-drug interactions, protein-protein interactions, and networks of effects based on similar biological pathways and cellular compartments were the aforementioned interactions. The integrations of this information might afford more detailed of drug effects and allow novel inferences for therapeutic strategies.