Implementation of Microservices Architecture for Application of Cyclooxygenase-2 Inhibitors Identifier

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Abstract. The identification of drug compounds that react to the body's cells is known as structure screening. This process can be assisted by a computer known as Structure-Based Virtual Screening (SBVS). This virtual screening process has been carried out by Istyastono for Cyclooxygenase-2 (COX-2). The screening process that has been carried out needs to be documented so that researchers can utilize for further research. Web-based applications with microservices architecture were chosen to develop a means of compound documentation because this application will be developed by bringing together two platforms, web and Linux shell script. An urgent need for this application to be built with the microservices architecture is the speed of application development for other enzymes based on this application. Application consist of web user interface, web service, data access and compound table. These components are mutually independent. Based on the results of implementation and discussion, the microservices architecture has provided guidance in developing applications so that applications are quickly built and easy to maintain and develop. It can be done because application is developed independently of each other.

1. Introduction
In the pharmaceutical field, the identification of drug compounds that react to the body's cells is an important initial stage in the drug discovery. To solve this problem, the pharmaceutical industry conducts a screening process of various drug compounds. Initially, this process was carried out in the laboratory, so it was expensive and took a long time. Currently, there are many computer-based or computing-based screening processes known as Structure-Based Virtual Screening (SBVS)[1].

This virtual screening process has been carried out by Istyastono for Cyclooxygenase-2 (COX-2) and managed to find the basic rules of screening that have been tested[2][3]. COX-2 enzyme has served as a target of choice in the development of anti-inflammatory drugs[4]. The screening process that has been carried out needs to be documented so that researchers can utilize for further research and web was the best documentation tools. There were many web development architectures and we chose microservices architectures as development framework because it offers speed of development. The microservices architecture appeared lately as a new paradigm for programming applications by means of the composition of small services, each running its own processes and communicating via light-weight mechanisms. This approach has been built on the concepts of SOA brought from crossing-boundaries workflows to the application level and into the applications architectures, i.e. its...
Service-Oriented Architecture and Programming from the large to the small[5]. The big motivation to perform a migration to a microservices architecture was an issue raised with on-demand capability that must meet the need for reusability, decentralized data governance, automated deployment, and built-in scalability[6]. Many organizations, such as Amazon, eBay, and Netflix, have solved complexity problem by adopting microservices architecture pattern. Instead of building a single monstrous, monolithic application, the idea is to split your application into set of smaller, interconnected services[7].

This research will produce an application that can perform the screening process and document the results. The challenge of this research is to combine two types of applications, namely web applications and Linux bash scripts. Another challenge is how to build the same application for different enzymes and can be built quickly in the future.

2. Methods
Basic algorithm of application can be seen in Figure 1. This algorithm is used for web-based application and does not have big different for mobile application. Input of application is a compound formula and the output are activation status of the compound.

![Figure 1. Basic algorithm of application in web-based platform](image1)

![Figure 2. Microservice for COX-2 Screening Application Design](image2)
Figure 2 describes the microservice deployment diagram of COX-2 screening consisting of simple applications. Initially, user use browser or mobile phone application to send compound formula and application will produce activation status of this compound. Browser application is built-in application such as Chrome, Firefox, Explorer, etc. Mobile phone application is custom application accessing Screening API Gateway in REST Service. Screening web UI and Screening API gateway will access Screening REST Service. We use Tomcat web service to deploy Screening REST Service and Screening API gateway. This service is very important service because it functions to access compound table and screening Linux shell script. For accessing compound table, this application use Hibernate framework. For compound screening itself, this application will execute Linux shell script that will analyse activation status of compound. The Linux shell script is developed based on Istyastono research[2,3]. We use the following softwares: OpenBabel8, SPORES1.3[9], PLANTS1.2[10], PyPLIF[11].

3. Result and Discussion

Figure 3 is a class diagram which is an implementation of design in Figure 2. Each class is implemented in different server/environment. Index.html class is a web user interface developed with HTML and javascript, executed in Apache web server. Index.html class call userCompoundService.java class, a web service, in form, http://url/getCompoundService. This web service is developed with Java and executed in Apache Tomcat server. This web service receive data in JSON form and will return output in JSON form. This service will check whether this compound is in the compound table. If it is exist, then this service will read the attribute / column result and the
reading result will be returned to index.html. If it doesn't exist, this service will call the compoundScreening.sh class.

Figure 4. Web based user interface of COX-2 Screening Application Design

Figure 4 shows result of COX-2 screening whether the text area will receive compound structure text and email user. Result of screening showed in bottom text area and formed in JSON.

Based on our experience, even though this application has not been completed yet, especially for mobile application, the application can provide results as expected. Application that are developed still have flaws in the shell program section and programmers just focus on completing the section. This fact also proves that microservices architecture is very helpful. This application can be accessed in http://it-projects.usd.ac.id/sbvs/index.html.

4. Conclusions
Based on the results of implementation and discussion, the microservices architecture has provided guidance in developing applications so that applications are quickly built and easy to maintain and develop. This result cannot be quantized because the application has not been completed. However, when viewed from the development side, the main framework of the application has been completed and just finish one part without changing the main framework. It can be done because application is developed independently of each other.

Further research and development can carry out the processing time in multiple screening so that performance will be measured. The addition of enzymes that will be screened also needs to be tried to observe whether there is a change in the main framework of the application.

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