PROGRAM BOOK AND ABSTRACTS

# International Symposium on Medicinal Plant and Traditional Medicine

# Indonesian Traditional Medicine for Human Welfare

Tawangmangu, June 4th - 6th 2014

Jointly organized by

BHAKTI HUSADA

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has participated in

The 46th Symposium of National Working Group of Indonesia Medicinal Plant
International Symposium on Medicinal Plant and Traditional Medicine
Theme: Indonesia Traditional Medicine for Human Welfare
4 - 6 June 2014, Tawangmangu, Indonesia, as:

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**Surat Keterangan**

Pengalihan Ijin Publikasi Mandiri

Kami, panitia pelaksana kegiatan ***International Symposium on Medicinal Plant and Traditional Medicine*** "Indonesia Traditional Medicine for Human Welfare", memberikan ijin Pengalihan Publikasi Mandiri secara online artikel dari:

Nama Penulis : Broto Santoso
Asal Institusi : Fakultas Farmasi Universitas Muhammadiyah Surakarta
Judul Artikel : **COMPARISON OF FREE DOCKING TOOLS**.

untuk dipublikasi secara Mandiri oleh yang bersangkutan. Artikel tersebut telah dipresentasikan secara poster dalam ***International Symposium on Medicinal Plant and Traditional Medicine*** "Indonesia Traditional Medicine for Human Welfare" yang diselenggarakan oleh Medicinal Plant and Traditional Medicine Research and Development Centre (MPTMRDC/B2P2TOOT) - NiHRD, Ministry of Health Republic of Indonesia in colaboration with National Working Group of Indonesian Medicinal Plant (POKJANASTOI)pada tanggal 4-6 Juni 2014 di Auditorium of Medicinal Plant and Traditional Medicine Research and Development Center (MPTMRDC/B2P2TOOT) Tawangmangu. Demikian surat ini dibuat agar dapat dipergunakan sebagaimananya mestinya.

Tawangmangu, 27 Februari 2015

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P-MPP-010

## COMPARISON OF FREE DOCKING TOOLS

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Database of natural medicinal compounds, primarily derived from plants are widely available, distributed and can be accessed for free via the Internet. The protein database that is responsible for a particular disease in molecular biology also has been established since 1971. Limited access of information on various results of research in Indonesia, repeatability of objects and topics of research are often the case, extract and fraction of medicinal plant resulted non-selective conclusion of target activity of disease, the lack of advanced research that gained successful outcome due to a very few in number of pure isolates that obtained from certain plants and many other difficulties that will be found in the development of Indonesian medicinal compounds. The insufficiency of research funding given decreased the amount of research and increased competition to getso as to the preliminary studies using prediction theory through computational chemistry is needed to rise the accomplishment of research, one of them is the virtual screening using docking tools. This study aimed to compare the docking tools is available for free. The parameters of comparison are simplicity of use, easiness of access to information, advantages and disadvantages for the novice user, the system that must be prepared, speediness for obtaining and analysing the results and the level of confidentiality. MarvinSketch and OpenBabel are main software that needed for supporting Docking tools. The selected docking tools must be available free for use online or offline. The use of online docking tools that provided by a third-party does not meet the desired level of confidentiality. Dock6, Dock3.7 and PLANTS are not stress-free in the installation or the docking procedure becauseit needs further experience concerning computer systems. PyRx, Chimera, MarvinSpace or VegaZZcould be selected as a candidate docking tools. They havean easy setup and operation as well as their trust worthy because they can be run offline. Chimera and PyRx recommended as docking tool that have to be used because it has the following advantages: both can be run on any operating system (Windows, Mac or Linux) and fulfil all the requirement. Application of database of natural medicinal compounds and proteintargetsusing docking tool: Chimera and PyRx should be recommended by the Indonesian government in order to become standard procedure of research before performing a certain activity assay of the plant as early prediction approaching the results to be acquired.

**Keywords:** Free Docking Tools, Chimera, PyRx, Dock6, PLANTS, MarvinSpace, VegaZZ, online, offline

P-MPP-011

## CHROMATOGRAM PROFILE (FINGERPRINT) KATUK LEAVES (*Sauropus androgynus* (L.) Merr) OF STANDARDIZATION AS A PLANT EXTRACT MATERIALS NATURAL MEDICINE

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Katuk (*Sauropus androgynus* L.) is a vegetable plant that is widely used in natural medicine products. To Prevent Counterfeiting Necessary components of the product to establish the standardization of quality simplicia/extract. This study aims to obtain a profile of the chromatogram (fingerprint) katuk leaf as the basis for standardization of extracts of natural medicine by identifying a mixture of natural medicines through the fingerprint (fingerprint). Results chromatogram profile (fingerprint) TLC analysis of the documentary system Obtained the best resolution to extract n - hexane, chloroform , ethyl acetate and methanol at λ 254 nm and λ 366 nm, visible light and the apparition anisaldehid ie spots with the mobile phase: n - hexane - chloroform - ethyl acetate (40:20:40) ; toluene - dioxane - acetic acid glacial (90:25:10), chloroform - acetone - formic acid (75:16:8) and cyclohexane - diethylamine - ethanol (60:30:10). Analysis by TLC-Scanner Obtain the best resolution of the ethanol extract, n -hexane, chloroform, ethyl acetate and methanol in the mobile phase

# Comparison of Free Docking Tools

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**Abstract**

Database of natural medicinal compounds, primarily derived from plants are widely available, distributed and can be accessed for free via the Internet. The protein database that is responsible for a particular disease in molecular biology also has been established since 1971. Limited access of information on results of Indonesian research, repeatability of objects and topics of research are often the case, extract and fraction of medicinal plant resulted non-selective conclusion of target activity of disease, the lack of advanced research that gained successful outcome due to a very few in number of pure isolates that obtained from certain plants and many other difficulties that will be found in the development of Indonesian medicinal compounds. The insufficiency of research funding given decreased the amount of research and increased competition to get so as to the preliminary studies using prediction theory through computational chemistry is needed to rise the accomplishment of research, one of them is the virtual screening using docking tools. This study aimed to compare the docking tools is available for free. The parameters of comparison are simplicity of use, easiness of access to information, advantages and disadvantages for the novice user, the system that must be prepared, speediness for obtaining and analysing the results and the level of confidentiality. MarvinSketch and OpenBabel are main software that needed for supporting Docking tools. The selected docking tools must be available free for use online or offline. The use of online docking tools that provided by a third-party does not meet the desired level of confidentiality. Dock6, Dock3.7 and PLANTS are not stress-free in the installation or the docking procedure because it needs further experience concerning computer systems. PyRx, Chimera, MarvinSpace or VegaZZ could be selected as a candidate docking tools. They have an easy setup and operation as well as their trustworthy because they can be run offline. Chimera and PyRx recommended as docking tool that have to be used because it has the following advantages: both can be run on any operating system (Windows, Mac or Linux) and fulfil all the requirement. Application of database of natural medicinal compounds and protein targets using docking tool: Chimera and PyRx should be recommended by the Indonesian government in order to become standard procedure of research before performing a certain activity assay of the plant as early prediction approaching the results to be acquired.

**Keywords:** Free Docking Tools, Chimera, PyRx, Dock6, PLANTS, MarvinSpace, VegaZZ, online, offline

## INTRODUCTION

Chemical compounds can be divided into two major groups. First, the natural group which to collect them through the isolation process of natural resource. Last, group of semi-synthesis that is produced by chemical synthesis or biosynthesis in the laboratory, but still their starting material derived from natural sources. Rapid developments of chemical technology have made more and more tools that are made to meet the needs of the chemical sources. The tools are held with the highest sensitivity, selectivity and toughness. Competitions of research for discovering new

entities compounds make scientists consciously collected millions of different compounds from the previous two groups of compounds. The discovery of new compounds from natural sources as a potential drug has attracted many investors to commercialize these databases of existing compounds.

Fortunately, databases of natural medicinal compounds, primarily derived from plants are widely available, distributed and can be accessed for free via the Internet. Some of them are NuBBE Database (http://nubbe.iq.unesp.br), Universal Natural Product Database (http://pkuxxj.pku.edu.cn/UNPD/), ZINC (http://zinc.docking.org/), PubChem (http://pubchem.ncbi.nlm.nih.gov/), ChemDB (http://cdb.ics.uci.edu), Chemspider (http://www.chemspider.com/), iScienceSearch (http://isciencesearch.com) and DistilBio (http://distilbio.com). Actually, there is an Indonesian portal for natural product database, but it is not quite satisfactory in supporting research. Indonesia has many natural sources of native plants.

Thus the protein database that is responsible for a particular disease in molecular biology also has been established since 1971, known as Protein Data Bank (http://pdb.org). This protein portal has collected more than a hundred thousand structures of protein, which are produced mainly using X-Ray Diffraction. Homology technique can be used as a method to get three-dimensional structure if the protein that needed was not found in existing database. A few of online service for protein modeling are the protein model portal (http://www.proteinmodelportal.org/) and SwissModel (http://swissmodel.expasy.org/). Modeller is one of many softwares that can do protein modeling offline. It can be downloaded and used for free with education license restriction.

Many Indonesian researchers have done good studies on topic of natural product, but information about their research results has been limited for others to access in real time. This occurred due to distance and lack of media to inform them as soon as possible. The information problem has consequences in a repeatability of objects and topics of research are often the case. In addition to the limitations of instruments, extract and fraction of medicinal plant resulted non-selective conclusion of target activity of disease. The lack of advanced research to acquire a successful outcome due to a very few in number of pure isolates that obtained from certain plants and many other difficulties that will be found in the development of Indonesian medicinal compounds. The insufficiency of research funding given, decreased the amount of research and increased competition to win so as to the preliminary studies

using prediction theory through computational chemistry is needed to rise the accomplishment of research. One of them is the virtual screening using docking tools. The first article about molecular docking has been published in year 1979. This study aimed to compare the docking tools is available for free.

## MATERIAL AND METHODS

Materials for testing are divided to hardware and software. MacBook Pro with Mac OS X Mavericks 10.9 has been chosen as hardware. Other operating systems (OS), i.e. Windows 7 and Linux (Ubuntu) have been built using virtualization technology. MarvinSuite and OpenBabel as main software to be installed and used for molecular docking. Both of them have the installer files for three kinds of operating system.

Some online docking tools have been selected, that are DockBlaster (http://blaster.docking.org/); SwissDock (http://www.swissdock.ch/docking/); ParDock (http://www.scfbio-iitd.res.in/dock/pardock.jsp); PatchDock, FireDock and FiberDock (http://bioinfo3d.cs.tau.ac.il/). Chimera (http://www.cgl.ucsf.edu/chimera/), PyRx (http://pyrx.sourceforge.net/), Dock6 (http://dock.compbio.ucsf.edu/DOCK_6/), Dock3.7 (http://dock.compbio.ucsf.edu/DOCK3.7/), PLANTS (http://www.tcd.uni-konstanz.de), VegaZZ (http://nova.disfarm.unimi.it) and MarvinSpace (http://www.chemaxon.com/) have been nominated as offline docking tools. The parameters of comparison are simplicity of use, easiness of access to information, advantages and disadvantages for the novice user, the system that must be prepared, speediness for obtaining and analyzing the results and the level of confidentiality. The selected docking tools must be available free for use online or offline.

## RESULTS AND DISCUSSION

Docking servers as the tools of molecular docking are available online and can be used free of charge. The availability of support facilities and ease of use of the docking server depends on the developer and docking software used. The user should first read the terms and conditions imposed by the developer and approved it before using the facilities of the docking server. The developers of docking servers usually attach manual along with sample files for the docking process. DockBlaster is managed by UCSF (University of California, San Francisco) using Dock3.5 program for workstations. Tutorial of DockBlaster use has been existed and new users are required to understand and be able to perform as required by the developer. The user should perform data preparation prior to docking. DockBlaster has 6 stages of docking that are

Preparer, Scrutinizer, Target Prep, Calibration, Docking and getting the Results. Any request of DockBlaster docking process uses a queue system (Figure 1). DockBlaster has provided a security (PIN number) to those who need it, but data that has been uploaded to DockBlaster is still opened and accessible to developers docking server itself. DockBlaster is not recommended for anyone who just begins molecular docking because the novice user must follow all the steps that are required without exception.

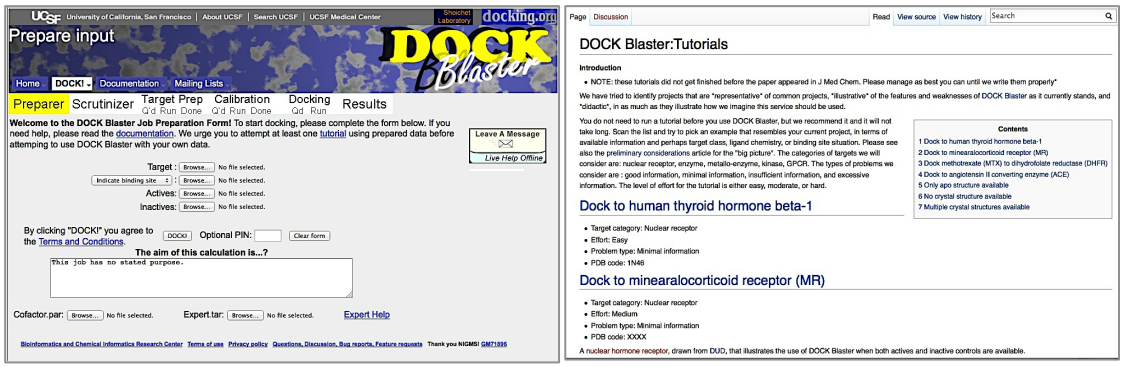


Figure 1. The homepage of DockBlaster (UCSF) and its tutorial page.

SwissDock is managed by the Swiss Institute of Bioinformatics. Stages of its molecular docking are simpler and easier to understand. SwissDock server is equipped with the facilities of searching and assistance that is very user friendly. ParDOCK is a docking server with a minimalist look. ParDOCK is a SwissDock lightweight version, but the capacity of the server is not good for online access (Figure 2).

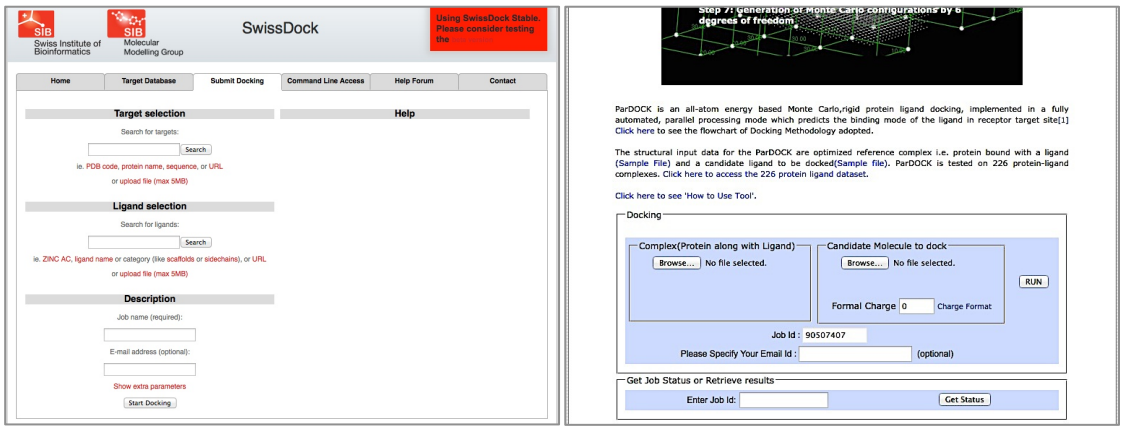


Figure 2. Graphical User Interface of SwissDock and ParDOCK for molecular docking

Wolfson's Structural Bioinformatics Group has also developed docking servers, some of which are PatchDock, FireDock and FiberDock (Figure 3). The homepage's Display of three servers is very simple but steps that must be done should be clarified very clearly. Among of these six examples that represent docking tools online, none of

them could convince users for the data that has been uploaded will not be abused for the profit of the group or its developers.

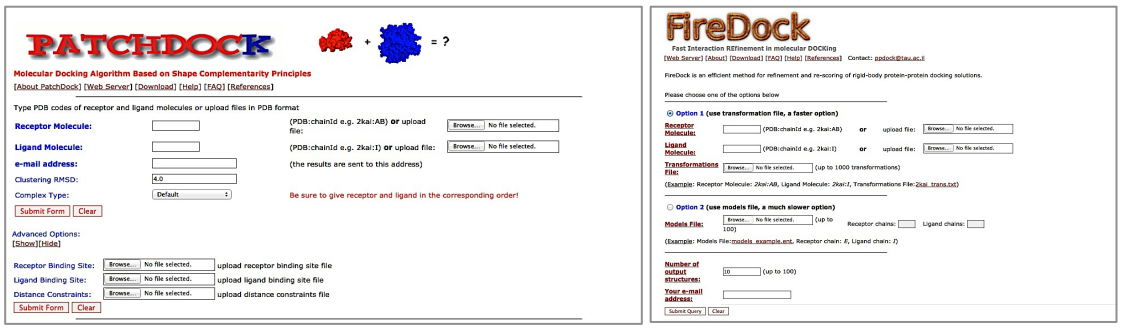


Figure 3. The front pages of PatchDock and FireDock from Wolfson's Structural Bioinformatics Group

Application of molecular docking can be done offline. Many free software that can be used and have the same quality calculations with existing commercial one. Obstacles to be faced are the level of ease of installation, the number of molecular docking steps that must be followed and the presence of other supporting software. Chimera can be installed on all operating system platforms, available for both 32bit or 64bit (Figure 4). Actually, Chimera is not a docking software but it is only the tools to run Vina, a real docking software. Docking steps in Chimera is a simple and guided way (Figure 5). Vina is only run for one molecul each session in Chimera.

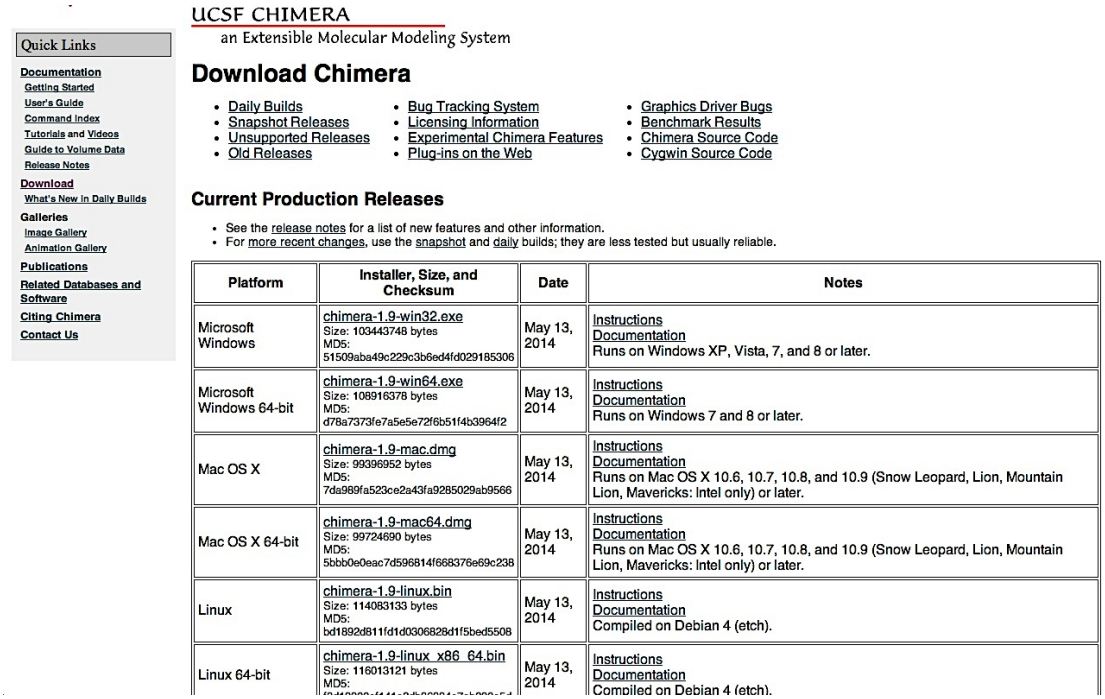


Figure 4. The download page of Chimera. The developer provides installer for all platform of operating system.

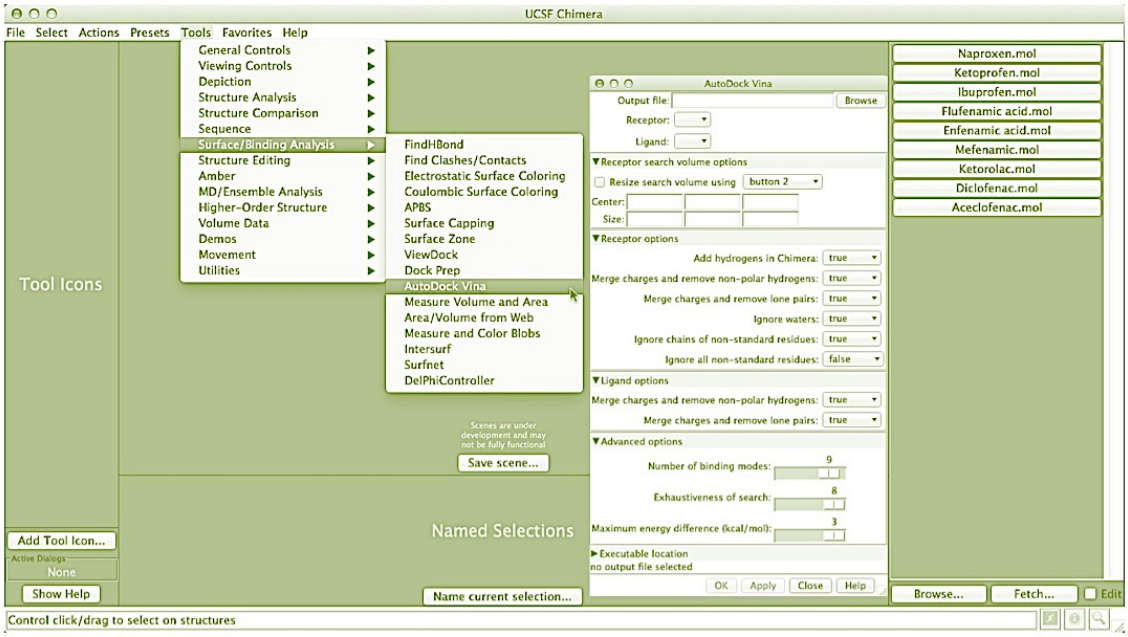


Figure 5. Window appearance of Chimera for Autodock Vina feature. Vina must be installed first if molecular docking will be done with offline session.

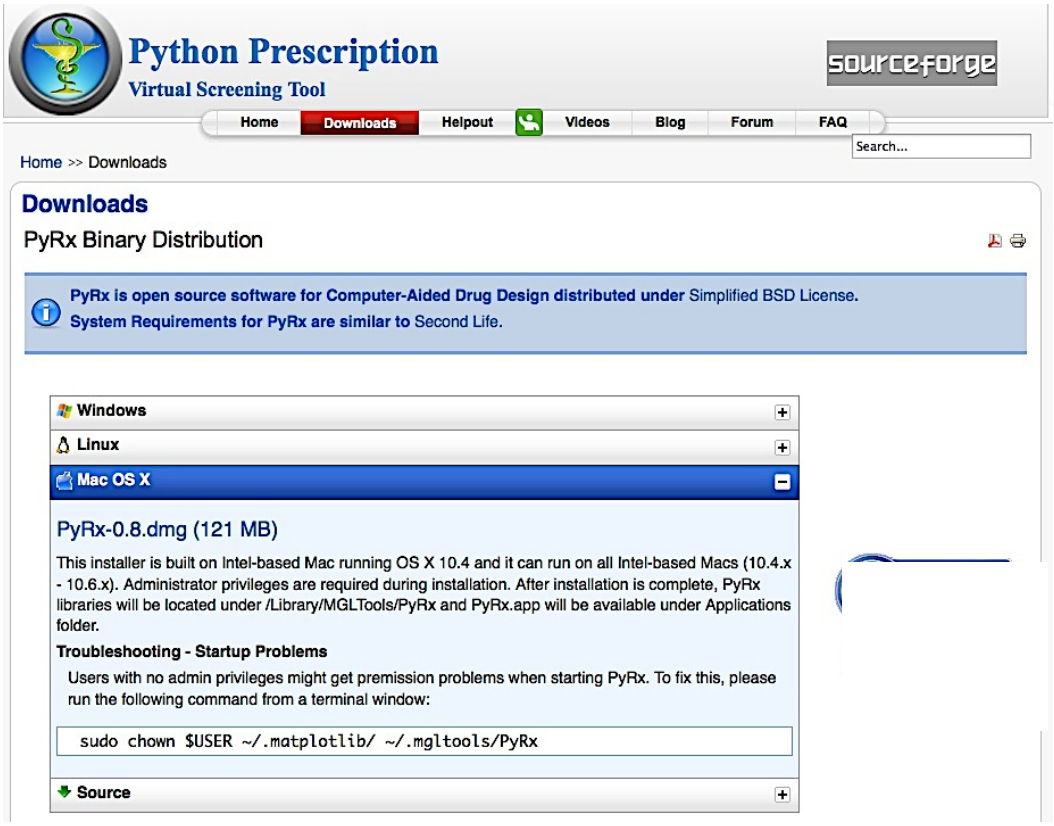


Figure 6. The download page of PyRx. The developer provides installer for all platform of operating system. Free version of PyRx that is available only till version 0.8.

Chimera weakness can be overcome by using PyRx. Molecular docking softwa-

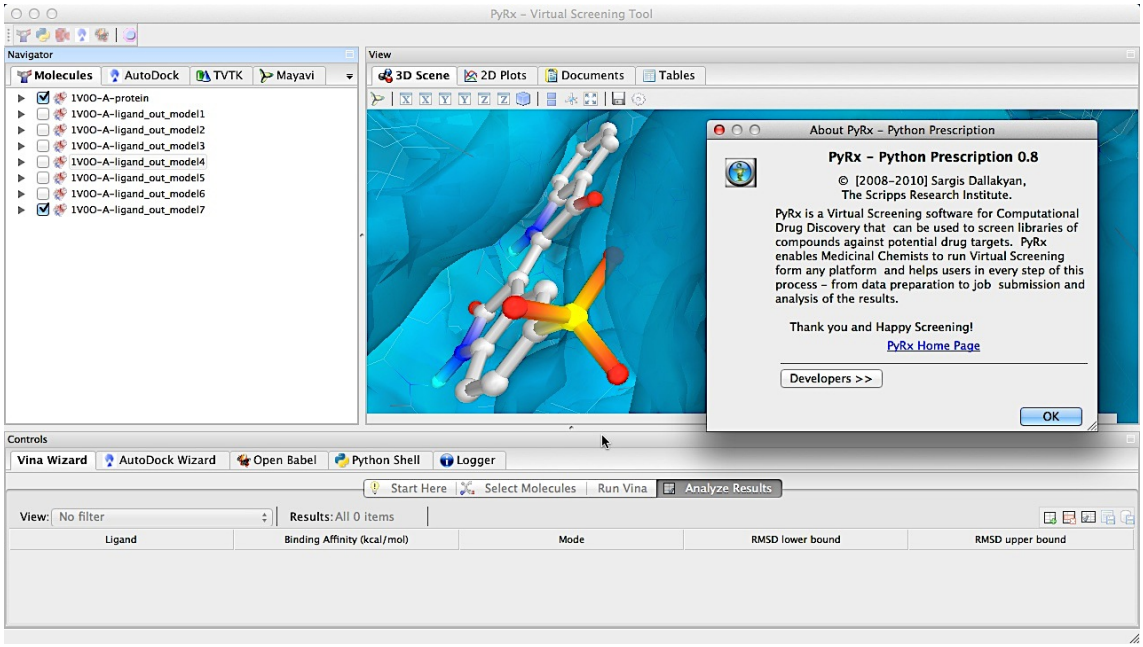


Figure 7. The workspace window of PyRx version 0.8 for Mac.

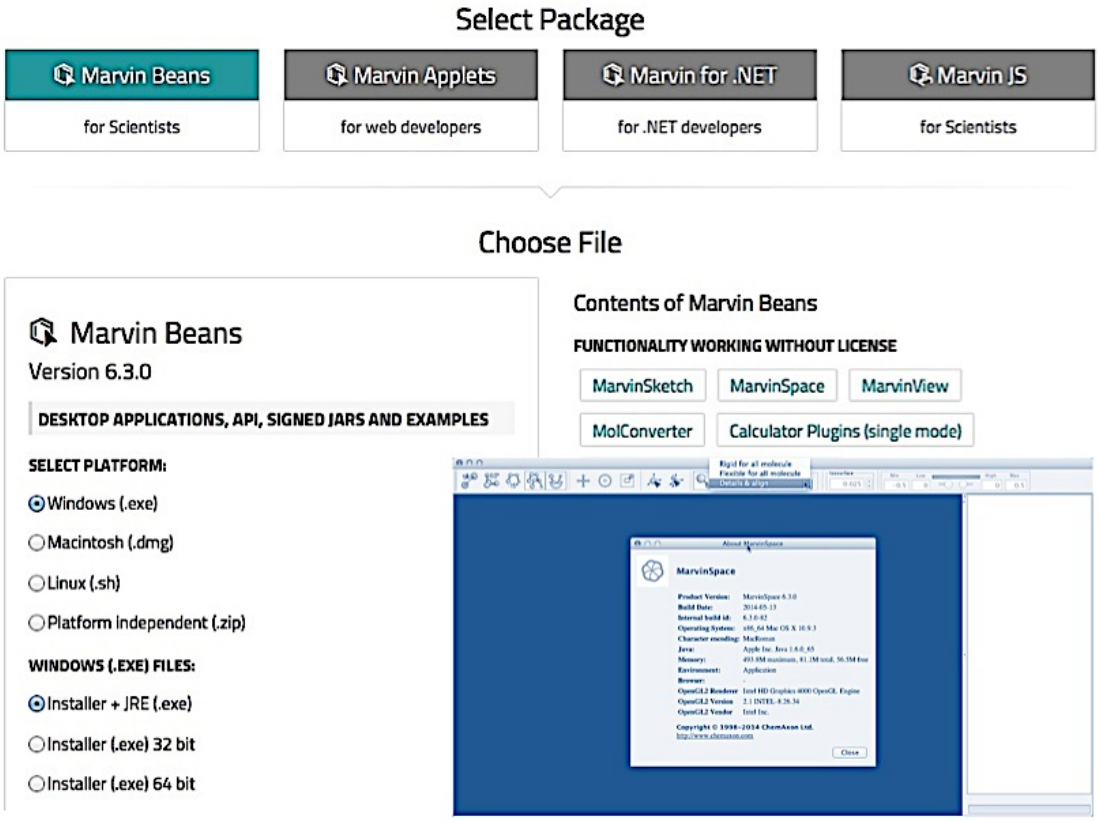


Figure 8. The download page of Marvin Beans program. The installer is provided for all platform of operating system. Blue box represents MarvinSpace's workspace.

re provided in PyRx is more complete, that are Vina and AutoDock. The program runs many compounds docking massively in one session. It is available free only up to

version 0.9 for Linux and version 0.8 for Windows and Mac (Figure 6). Its feature is still not user friendly for the visualization of docking results and cannot involve water directly with the software. Unfortunately, free version of PyRx does not offer the input feature for the center gridbox and its size manually. These facilities can be enjoyed at paid version of PyRx. The workspace of PyRx shown in Figure 7.


Figure 9. The download page of VegaZZ installer. The installer is only provided for Windows system.

Other tools that is good to try for docking are MarvinSpace and VegaZZ. Marvin Space is free for any platform, but it is very simple command and has many other limited features (Figure 8). VegaZZ can only be operated on one native platform operating system as the same as DOCK and PLANTS. They have high level of difficulty to operate. DOCK is intended to expert person who wants to run molecular docking.

The use of online docking tools that provided by a third-party does not meet the desired level of confidentiality. Dock6, Dock3.7 and PLANTS are not stress-free in the installation or the docking procedure because it needs further experience concerning computer systems. PyRx, Chimera, MarvinSpace or VegaZZ could be selected as a candidate docking tools. They have an easy setup and operation as well as their

trustworthy because they can be run offline. Chimera and PyRx recommended as docking tool that have to be used because it has the following advantages: both can be run on any operating system (Windows, Mac or Linux) and fulfil all the requirement.

Table 1. Comparison of offline or online Docking Tools

| Name of docking tools | OS Platform | Installation Step | Usage Step | Notes | Security |
|---|---|---|---|---|---|
| Online tools | | | | | |
| DockBlaster | all | - | expert | Difficult to understand | private but not secure |
| SwissDock | all | - | moderate | Instruction is easy to follow | private but not secure |
| ParDock | all | - | moderate | - | private but not secure |
| PatchDock, FireDock, FiberDock | | - | moderate | - | private but not secure |
| Offline tools | | | | | |
| Chimera (vina) | all | easy | moderate with GUI | Good visualization repeatable | private and secure |
| PyRx (AutoDock-vina) | all | easy | moderate with GUI | Visualization is not good Free version cannot repeatable | private and secure |
| Dock6 | unix | expert | expert without GUI | Not recommend for novice user | private and secure |
| Dock3.7 | unix workstation | expert | expert without GUI | Not recommend for novice user | private and secure |
| PLANTS | all* | moderate | expert without GUI | Not recommend for novice user | private and secure |
| VegaZZ | windows | easy | expert with GUI | Hard to understand | private and secure |
| MarvinSpace | all | easy | moderate without GUI | Limited feature | Private and secure |

## CONCLUSION

Application of database of natural medicinal compounds and protein targets using docking tool: Chimera and PyRx should be recommended by the Indonesian government in order to become standard procedure of research before performing a certain activity assay of the plant as early prediction approaching the results to be acquired.

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