The potential of in-silico approach to support government programs to achieve eco-friendly agriculture: Studies on urban agriculture

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Abstract. As one of the supporters of sustainable development is an effort to fulfill food needs realized through the agricultural sector. However, the current agricultural system mostly uses chemical pesticides, especially in urban agriculture. This is done as an effort to maintain agricultural production and fulfill food needs in urban areas. Even though food needs are met, food security is not yet fulfilled. In solving this problem, the Indonesian Government has created a program that aims at agricultural development, namely Eco-friendly agriculture. Regarding Law Number 22 the Year 2019 Article 48 Concerning Integrated Pest Management, which provides directions such as counseling on Eco-friendly agriculture. In this case, the bioactivity of organic pesticides or biopesticides is the main factor of agriculture. The study is carried out by the Technical Implementing Unit to conduct trials to obtain suitable organic pesticides. The in-silico approach can be used as one of the primary methods to support Government programs. This approach can be used to simulate drug discovery and to determine its bioactivity by performing molecular docking. This study concludes that the in-silico approach has the potential to support Government programs to realize Eco-friendly agriculture as an initial technical effort of the program.

1. Introduction

The understanding provided by sustainable development includes the economic and environmental order and considers the social order. The main objective of sustainable development shows that meeting the needs that are being pursued today without sacrificing the ability of future generations to meet their needs [1]. Economic, environmental, and social arrangements are needed in terms of food security. Agricultural sustainability that focuses on the environment needs to be considered systematically by revealing the relationship between aspects of sustainability [2]. Food and agriculture sustainability is one of the goals of sustainable development which is always associated with biodiversity, health, innovation, and technology transfer [3].

The agricultural sector has a significant role in meeting our food needs. The food needs will increase in line with the increasing population worldwide, which is estimated to increase to 9 billion by 2050 [4]. The agricultural model that is still attached to the farmer’s mindset is the farm process by prioritizing chemical pesticides. This occurs because pesticides are considered an essential component of a comprehensive strategy to meet increasing demand and prevent losses [5]. In general, pesticides are used to keep plants healthy and to avoid disease and plant pests. Pesticide products have market rules in marketing, such as cannot be marketed without a license. Besides, an evaluation that includes an assessment of environmental and health risks is related to the law of agriculture [6]. The potential
to communicate and encourage the implementation of practices to reduce environmental impacts is the collaboration between the Government and farmers who are the main actors in agriculture.

Development in the agricultural sector is essential and must be proportional to the total population to meet the food demand [7]. One system that focuses on empowering and giving farmers the ability to make the right decisions to solve agricultural problems in agricultural extension. In general, agricultural extension in developing countries such as Pakistan aims to solve production and crop management problems [8]. The food conveyed the Indonesian Government's efforts to participate in technical agricultural management and Agricultural Security Service as an integrated pest control system based on Law Number 22 the Year 2019 Article 48 concerning Integrated Pest Management with programs as field school (SLPHT). One of the programs carried out in the SLPHT activity was to increase farmers' insights and knowledge about eco-friendly agricultural technology. This is done by conducting training and improving skills to make biopesticides and organic fertilizers. Biopesticides and organic fertilizers submitted are researched and tested first by the Plant Protection Agency. Apart from that, the program also includes assistance in biopesticides and organic fertilizers [9].

The Government program in the form of SLPHT is also applied to urban agriculture in Jakarta. One of the sub-districts maintained as zoning of paddy farming following the Regional Regulation of the Special Capital Region of Jakarta Number 1 of 2014 about Plan Details and Zonation Regulations Article 438 is Cakung Subdistrict, East Jakarta. Urban agriculture is closely related to economic development issues, especially in developing countries. Urban agriculture is seen as a lifesaver of the economy, helping to provide food and livelihoods [10]. The transition to support a production-based economy with natural ingredients is a viable one economically and technologically and socially expected. Apart from the need for support from experts and policymakers, it requires acceptance and involvement from consumers in a transition [11]. Alternatives to substitute non-renewable resources will create a balance with ecological limits. However, the conventional method with multiple trials involves many components, much time, and high cost. This is relatively inefficient due to frequent failures.

The in-silico approach can support a viable transition to eco-friendly agriculture in urban areas by contributing to predicting the bioactivity of biopesticides. The in-silico approach through molecular docking is an alternative or breakthrough to attract farmers to use biopesticides. The in-silico approach is carried out based on theoretical results that are translated into a computer program in the form of a docking application [12] to shorten discoveries. In general, molecular docking performs position searches with flexible ligand patterns and rigid proteins. Each position is assessed based on its shape and characteristics to find the most appropriate area.

Given the challenges faced by the Government in realizing Eco-friendly agricultural programs, in addition to the in vitro practices that have been carried out by the Government and farming actors, the in-silico approach has the potential to support eco-friendly agriculture. Besides its ability to predict bioactivity, the in-silico approach could also shorten the discovery and costs involved. It is hoped that the literature studies which show the effectiveness of the in-silico approach can be used as an effort to support Government programs to realize eco-friendly agriculture with cost-effective and production materials.

2. Method
The method used in this research is in-depth interviews and literature studies. In-depth interviews were chosen as one of the ways in this study to show eco-friendly agriculture as an ongoing Government program in Jakarta. In-depth interview informants are Government actors as informants who understand Government programs on eco-friendly agriculture. The literature study was chosen to show that ongoing Government programs could potentially be supported by an in-silico approach as the first step before an in vitro approach. This aims to show that the in-silico approach can be used in agriculture.
2.1. Data collection
Information related to government programs on eco-friendly agriculture was obtained through in-depth interviews with government actors. Two informants were chosen to represent the respondents who expressed the government actors, namely those for agricultural control and agricultural technical implementers. In-depth interviews were chosen because they were considered as an all-knowing participant who knows the current plans and systems regarding government programs. The selected informants were government actors related to agricultural activities in Jakarta. The question to know about government programs includes 1) program grand plans; 2) actors who play a role; 3) ongoing activities. After learning the overall government program, the researcher tries to link it with the in-silico approach, which has the potential to support current programs.

2.2. Article review and analysis
The literature study on the in-silico approach was carried out on research that utilizes the in-silico approach in agriculture. The results of the in-silico approach through docking applications can help understand the benefits of molecular docking demonstrated by ligand and macromolecular interactions. The results of these interactions show the benefits of the in-silico approach by predicting the bioactivity value between the ligands and macromolecules tested. After knowing the benefits of the in-silico approach in agriculture and government programs on agriculture, the researcher conducted a descriptive analysis by linking the in-silico approach that can support current agricultural programs.

3. Results and discussion

3.1. Eco-friendly agriculture as a government program
This information was taken from government actors about government programs includes 1) program grand plans; 2) ongoing activities, and 3) actors who play a role. The informants stated that the Government's big plans for agriculture in Jakarta were:

“Our direction is actually towards agricultural development, agricultural development means that we minimize the use of chemical substances that might pollute the environment. Especially the food itself...” (Informant 1)

The statements from the informants indicated that the government program was aimed at sustainable agriculture through eco-friendly agriculture programs. This is supported by the activities carried out, as stated by the speakers:

“... so that we minimize the use of pesticides, nah for pest and disease control, we reduce the use of chemical pesticides so we switched to a plant-based pesticide use.” (Informant 2)

The information provided by the informants shows that eco-friendly agriculture which was initiated in the development of agriculture is meant as one of the government’s efforts to contribute to the technicalities of agricultural management. Organic pesticides that are considered more eco-friendly are used to replace the use of chemical pesticides that produce residues. In accordance with the Food, Maritime and Agricultural Security Service, the government conducts agricultural extension as an integrated pest control system which is based on Law Number 22 the Year 2019 Article 48 concerning Integrated Pest Management, known as field schools. In accordance with Al-Zahrani et al. (2019), agriculture program gives farmers the ability to solve environmental problems with an eco-friendly approach.

Ongoing programs on agriculture can be achieved by the existence of cooperation between farmers or government. Actors who play a role in supporting the running of eco-friendly agriculture programs are the Technical Implementation Unit, namely POPT officers both in the region and laboratories as
well as farmers. They are directly related to agricultural activities. This is supported by the information from an informant who said:

“So, to encourage farmers or actors who produce vegetables to use organic pesticides, so in UPT they are assigned to produce organic pesticides. Because there is the name of the UPT supervisor, in the Protection office ... later the operation will be at the Technical Implementing Unit.”

(Informant 1)

The programs initiated by the government regarding agricultural activities are efforts to fulfill food needs and food security. The laboratory assists the realization of this program in producing organic pesticides such as Trichokompos, according to Figure 1, which has its function to improve plant health, control pathogens, increase plant growth and production, and become a soil repairing medium. Also, Trichokompos can be applied in nurseries as essential fertilizers and additional fertilizers to be useful as plant protection.

![Trichokompos](image)

**Figure 1.** Trichokompos produced by the laboratory (agricultural section).

Organic pesticides produced by the laboratory as a technical implementation unit are a form of Government efforts to reduce environmental pollution. Given that urban agriculture in urban areas must be able to meet the food needs of an increasing population. This is in accordance with Tripathi and Maktedar (2019) that the importance of developing agricultural activities must be proportional to the community to meet food demand. Food security is also considered necessary because it includes consumer health. This is in accordance with Bannerman (2020), who said that food sustainability which achieved through agriculture is often associated with health, innovation, biodiversity, and technology transfer.

3.2. *In-silico* approach to agricultural activities

Previous research has proven that in addition to being used as a cosmetic product, the *in-silico* approach can also be used in agriculture. The study demonstrated the bioactivity of the interactions
that occur in selected ligands and macromolecules. The use of the *in-silico* approach that has the potential to support eco-friendly agriculture is shown in Table 1.

**Table 1.** Molecular docking studies in the agricultural sector.

| Title                                                                 | year | Result                                                                                           |
|-----------------------------------------------------------------------|------|--------------------------------------------------------------------------------------------------|
| Localization and *in silico* study of the vegetative insecticidal proteins Vip2S-Vip1S of *Bacillus thuringiensis* | 2016 | The 3D model of Vip2s or *Bacillus cereus* with the access code from PDB that is 1QS1 is tested for toxicity using the Swiss Model protein structure homology modelling server. Modelling using the *in-silico* approach shows that the 3D structure of Vip2s is a mixture of α / β protein. The resulting bioassay showed weak toxicity against lepidopteran *Spodoptera littoralis* [13]. |
| *In silico* identification of new potentially active brassinosteroid analogues                                           | 2018 | One of the hormones found in various plant species is brassinosteroids (BRs). BRs function as strong growth promoters and come from valuable natural sources and are a limitation. The *in-silico* approach was carried out by simulating the molecular docking of 20 synthetic steroids, which was carried out by contact-based analysis, exposure levels of polar groups to the solvent and binding affinity. The results showed that 17 out of a total of 20 steroids could potentially activate the BRI1 receptor, which leads to increased growth or resistance to biotic and abiotic stresses associated with agronomy [14]. |

Molecular docking studies are conducted to help the agricultural sector to show that the *in-silico* approach can be used as a useful additional method. Localization and *in-silico* study of the vegetative insecticidal proteins Vip2S-Vip1S of *Bacillus thuringiensis* showed that using the *in-silico* approach showed the toxicity of Vip2s is a mixture of α / β protein against the weak lepidopteran *Spodoptera littoralis*. Then, the *in-silico* approach can also be used for simulations of obtaining steroids that have the potential to support plant growth, as shown in Morena-Castillo (2018) research.

Food production improvement to meet food needs and protect global populations as well as the efforts to control disease vectors for insect control can be done by using the *in-silico* approach. The approaches used in the discovery of organic pesticides are as diverse as the bioactive hypothesis and natural products. The industry widely uses *in-silico* approach as a virtual input modelling. The screening carried out in the *in-silico* approach focuses on the compounds found in certain plants and insect pests. The potential input is done virtually on the model of the receptor or target enzyme. This approach aims to increase the likelihood of finding new active ingredients and minimizing the number of compounds that need to be synthesized. According to Sparks et al. (2019) *in-silico* approach serves as an attempt to predict bioactivity and potentially increase the possibility of finding new active ingredients. This study shows that *in-silico* approach can support Government programs with the efforts to predict early production of organic pesticides by reducing trial and error in the use of synthesized materials. So, it can be said that besides accelerating the experimental process as the first step of technical support for eco-friendly agriculture programs initiated by the Government, *in-silico* approach can also reduce the materials used for trial and error so that economically, the *in-silico* approach is an efficient and effective method. [15]

**4. Conclusion**

From the in-depth interviews and literature review conducted, it can be concluded that the Government program for Eco-Friendly Agriculture is one of the efforts made to reduce environmental pollution due to the use of pesticides using biopesticide alternatives. The *in-silico* approach used by
the industrial sector can also be used in the agricultural sector. The in-silico approach has the potential to support Eco-friendly Agriculture programs in the early technical part as a trial of the experiment and formulation discovery steps. This effort can facilitate the process of experimentation and simulation for Eco-friendly agriculture. Besides, the in-silico approach can support agricultural extension activities as an integrated pest control system based on Law Number 22 the Year 2019 Article 48 concerning Integrated Pest Management as a basic simulation of analogy.

Acknowledgements
This research is funded by Penelitian Tesis Magister Kementerian Riset dan Teknologi/Badan Riset dan Inovasi Nasional (KEMENRISTEK/BRIN)—Universitas Indonesia with contract number 8/E/KP.PTNBH/2020 and 255/PKS/R/UI/2020.

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