

## STUDY OF COMPUTATION AND PHYTOCHEMICALS CONTENT IN TEMULAWAK (*CURCUMA XANTHORRHIZA*) AS ANTIBACTERIA

Hana Safitri<sup>a</sup>, Fadil Alfarisi<sup>b</sup>, Nadia Marsila<sup>c</sup>, Dina Lisyanti<sup>d</sup>

<sup>a</sup>Magister Program of Biochemistry, Postgraduate, Central Luzon State University, Nueva Ecija, Philippines

<sup>b</sup>Department of Chemistry, Faculty of Mathematics and Science, Padang State University, JL. Prof. Dr. Hamka, West Freshwater, North Padang, Indonesia, 25171 Indonesia

<sup>c</sup>Magister Program of Educational Chemistry, Postgraduate, Padang State University, JL. Prof. Dr. Hamka, West Freshwater, North Padang, Indonesia, 25171 Indonesia

<sup>d</sup>Magister Program of Educational Chemistry, Postgraduate, Jambi University, JL. Jambi Out of Town, Muaro Jambi, Indonesia, 363611 Indonesia

\* Corresponding email: fadilalfarisi12@gmail.com

### ABSTRACT

Infectious diseases are still a public health problem, especially for developed and developing countries. Including in Indonesia health problems are one of the big problems. One of the causes is infection from bacteria. To fight diseases caused by these bacteria, antibiotics or antibacterials are needed. The content of curcumin and curcuminoids in temulawak (*Curcuma xanthorrhiza* Roxb) has various benefits, including antioxidant and antibacterial. The content of curcumin and curcuminoids in temulawak is considered capable of inhibiting the growth of disease-causing bacteria. From the computational study of the phytochemical content in temulawak as an antibacterial, the curcumin content in temulawak (*Curcuma xanthorrhiza* Roxb) has an inhibitory effect on *staphylococcus* bacteria.

**Keywords :** Ginger (*Curcuma xanthorrhiza* Roxb), Cancer, Curcumin and Demetoxicurcumin.

### 1. INTRODUCTION

Diarrhea is a condition in which a person defecates with a soft or liquid consistency [1][2][21]. Diarrhea is a clinical disease in which diarrheal disease is grouped into 6 groups of infections caused by bacteria, viruses and parasite infections [3][4][22]. Classification of diarrheal diseases in several types based on the disease, namely: (1) diarrhea due to viruses such as rotavirus and adenovirus [5][23], (2) invasive bacterial diarrhea, (3) parasitic diarrhea caused by protozoa such as *Entamoeba histolytica* and *giardia lamblia*[6], (4) diarrhea due to illness (5) diarrhea due to drugs [25], (6) diarrhea due to food poisoning [7][8][24].

Diarrhea is the number one cause of death in infants (31.4 %) and in children under five (25.2%), while in all age groups it is the fourth leading cause of death with a percentage (13.2%)[9][10][11] The number of extraordinary events (KLB) in diarrhea sufferers in 2013 was 646 cases [12][26]. The highest mortality rate due to diarrheal outbreaks occurred in North Sumatra, namely 11.76 % [13][14].

Temulawak has antimicrobial effects against several microorganisms, especially against bacteria *Bacillus subtilis*, *Escherichia coli*, and *Staphylococcus aureus* [15][16][27]. In addition, ginger can also have an effect on fungi so that it can be useful as an antifungal, examples of fungi that can be affected by ginger are *Saccharomyces cerevisiae*, *Aspergillus niger*, and *Penicillium notatum* [17][18][28]. The purpose of making this template is to understand the benefits of ginger and what bacteria it can treat in diarrheal disease that can affect all humans [29]. And what are the elements contained in this temulawak plant that are beneficial for humans? human [19][20][30].

## 2. LITERATURE REVIEW

Cancer is a disease caused by abnormal growth of body tissue cells, resulting in death with the number of sufferers increasing every year. One of the groups of diseases that are often suffered by the community is disorders of the digestive system, which starts from the mouth to the sewer. Several types of diseases included in this group include diarrhea, constipation, stomach pain, ulcers, constipation, canker sores, sore mouth, excessive gas discharge, toothache and hemorrhoids. Some data show that disorders of the digestive system are a serious problem and need immediate treatment.



**Figure 1.** Curcuma

Another benefit of temulawak (*Curcuma Xanthorrhiza*) is to refresh the body, accelerate metabolism, healthy liver function, increase appetite, as an immunomodulator and hepatoprotector. And temulawak (*Curcuma Xanthorrhiza*) is also used to increase endurance and stamina. Temulawak extract (*Curcuma Xanthorrhiza*) can induce immune system activity, administration of temulawak

(Curcuma Xanthorrhiza) can increase immune response in chickens given the bird flu vaccine. The use of temulawak (Curcuma Xanthorrhiza) in traditional medicine is widely used in the treatment of digestive disorders, jaundice, vaginal discharge, increases endurance and maintains immunity. health.

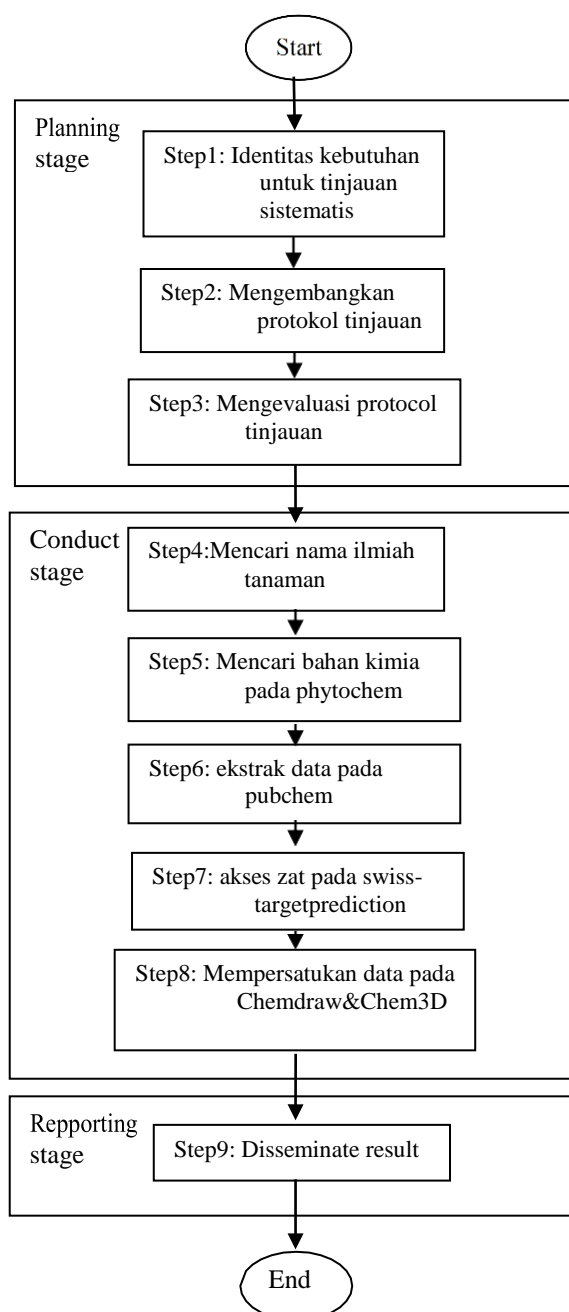
### 3. EXPERIMENTAL

Hardware, Software and Webserver This study uses a literature review method or the SLR (systematic literature review) approach to review studies, assess and interpret and gather information about the compounds contained in white turmeric and their role in helping cure cancer.

Personal hardware Acer core i3 laptop, the software used [is https://phytochem.nal.usda.gov/phytochem/search](https://phytochem.nal.usda.gov/phytochem/search), <https://pubchem.ncbi.nlm.nih.gov/>, <http://swisstargetprediction.ch/> The analyzed material was obtained from the Phytochem database taken from the Pubchem database. Material analysis was carried out on swisstarger prediction to see the content contained in Curcuma

Furthermore, the plant was researched by Dr. Duke's Phytochemical and Ethnobotanical Database with scientific name Curcuma zanthorrhiza. The search was aimed at looking at the chemicals in it, where the author took Curcuma zanthorrhiza and got the chemicals curcumin, D-champor, and Desmethoxycurcumin. After that, one by one the chemical was extracted and the compound elements in Isomeric SMILES were extracted then enter the element of the compound in Swisstarget prediction to see which percentage of the compound contains the most. The next step is to copy the IUPAC Name in Pubchem earlier, and access to Chemdraw and make optimizations with Chem3d to see the 3D structure image and how much energy is generated.

The last step is the disseminate result, which from the chemical obtained from swisstarget prediction, the results are curcumin, D-champor, Desmethoxycurcumin and Desmethoxycurcumin. Where in curcumin contains 20% oxidoreductase, 6.7% membrane receptor, 6.7% writer, 20% enzyme and 6.7% protease. Meanwhile, D-champor contains 23.3% nuclear receptor, 20% oxidoreductase, 20% enzyme, 6.7% protease, and 13.3% secreted protein. And desmethoxycurcumin contains 20% oxidoreductase, 20% enzyme, 6.7% protease and 6.7% membrane receptor.



**Figure 2.** Systematic Diagram

## 4. RESULTS AND DISCUSSION

### 4.1 Result

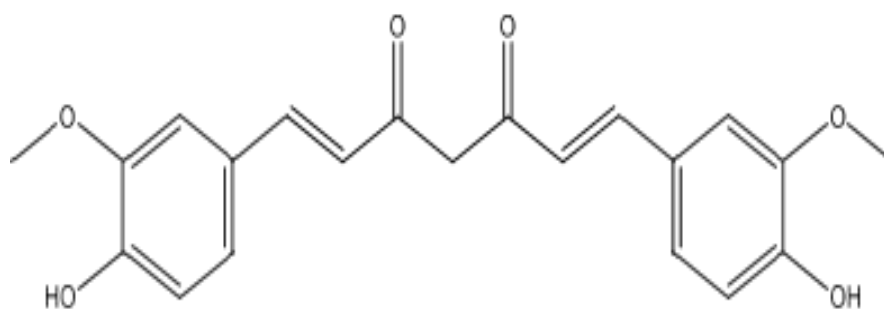
This research is viewed from the number of people who experience cancer. For cancer prevention, regular physical exercise is recommended, increasing physical activity such as walking to work, using stairs instead of elevators, and gardening. Physical exercise can reduce the risk of breast, colon, and endometrial cancer, as well as provide physical and mental benefits for cancer patients.

Regular physical activity plays a role in cancer prevention by maintaining ideal body weight, regulating sex hormones, insulin, prostaglandins, and having a good effect on the immune system. immune.

Energy balance is an important factor in reducing susceptibility to cancer because of its indirect effect on insulin levels, insulin-like growth factor-I (IGF-I), and various inflammatory markers.<sup>13</sup> Low vitamin D levels are responsible for risk cancer.

In overcoming cancer, the author wants to inform the public of the importance of exercise and consuming healthy foods to avoid cancer. Where cancer is one of the deadliest diseases in the world. The compounds contained in temulawak have 9 chemical compounds that have a charge, but which can be tested or seen in chemdraw ultra and chemdraw 3D, there are 3, namely:

1. Curcumin



**Gambar 1.** (1*E*,6*E*)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione

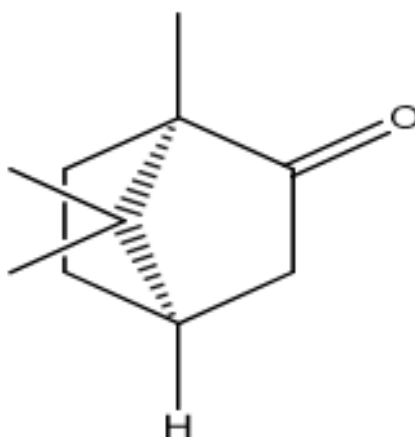


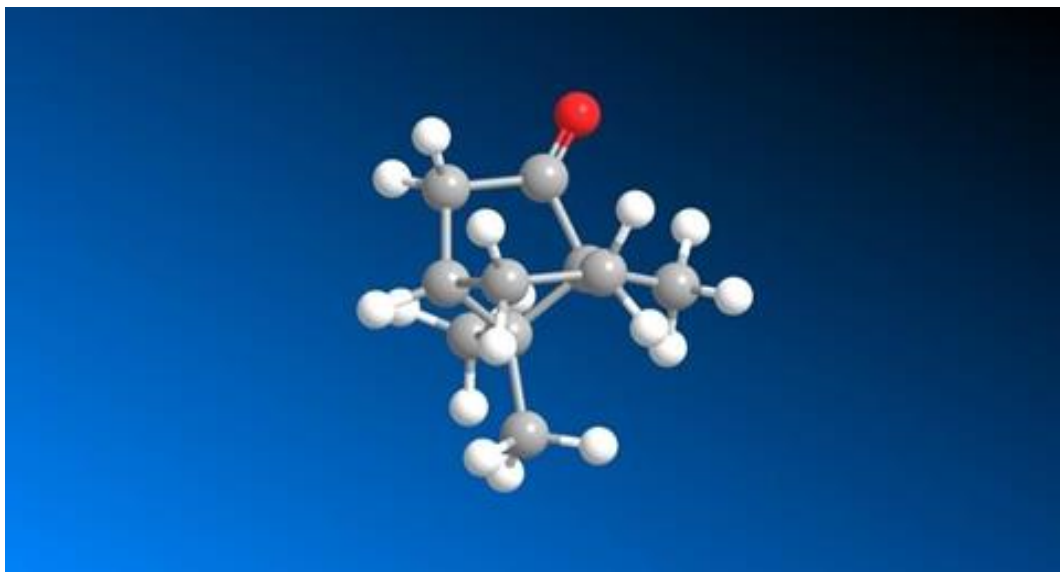
**Gambar 3.** Before being optimized

Atom	X(A)	Y(A)	Z (A)
C(1)	21.023	36.775	- 0.8777
C(2)	11.093	28.120	- 0.6486
C(3)	- 0.1759	32.140	- 0.7576
C(4)	- 12.966	22.372	- 0.4990
C(5)	- 0.7181	0.8907	- 0.1393
C(6)	- 15.398	- 0.1459	0.1357
C(7)	- 10.273	- 13.389	0.4544
O(8)	- 0.4279	43.555	- 10.622
O(9)	0.4796	0.7396	- 0.0972
C(10)	- 18.405	- 23.647	0.7266
C(11)	- 13.058	- 36.093	10.591
C(12)	- 21.542	- 46.795	13.429
C(13)	- 35.372	- 45.050	12.943
C(14)	- 40.719	- 32.604	0.9619
C(15)	- 32.235	- 21.902	0.6780
O(16)	- 16.348	- 58.886	16.658
C(17)	- 22.536	- 69.089	0.9297
O(18)	- 43.613	- 55.446	15.700
C(19)	33.741	32.796	- 0.7697
C(20)	44,100	41.825	- 10,088
C(21)	57,369	37,674	- 0.8963
C(22)	60,278	24,493	- 0.5446
C(23)	49.9	15.4	-

**Figure 4.** Cartesian table

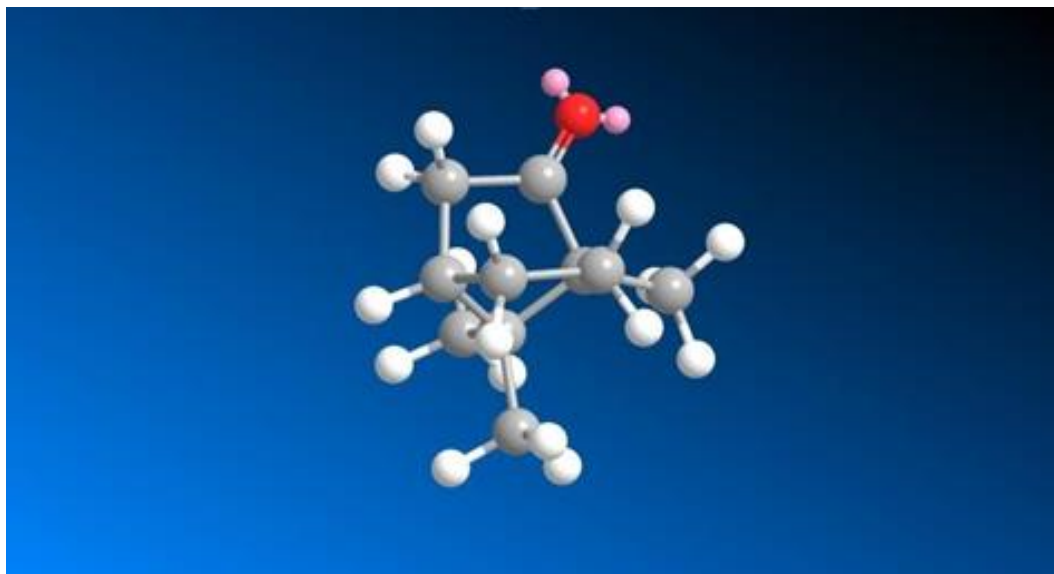
## 2. D-champor

**Figure 5.** (1 *R* -4 *R* )-1 ,7,7 -trimethylbicyclo[2.2.1]heptan-2-one

**Figure 6.** Before Optimization

Atom	X(A)	Y(A)	Z(A)
C(1)	- 15.849	0.3901	- 0.1040
C(2)	- 22.330	17.370	- 0.4668
C(3)	- 36.610	15.903	0.0800
C(4)	- 36.538	0.1776	0.6882
C(5)	- 27.956	0.1913	19.646
C(6)	- 13.676	0.3380	14.177
C(7)	- 27.525	- 0.5787	- 0.2871
O(8)	- 17.401	26.787	- 10.407
C(9)	- 32.945	- 0.6062	- 17.101
C(10)	- 25.097	- 20.637	- 0.0513
C(11)	- 0.3014	0.1345	- 0.8830
H(12)	- 46.806	- 0.2110	0.8713
H(13)	- 38.726	23.588	0.8567
H(14)	- 44.454	17.298	- 0.6972
H(15)	- 29.102	- 0.7584	25.337
H(16)	- 30.788	0.9993	26.757
H(17)	- 0.8927	12.747	17.861
H(18)	- 0.6885	- 0.4843	17.365
H(19)	- 33.264	- 16.571	- 20.753
H(20)	- 43.218	- 0.1780	- 17.235
H(21)	- 26.318	- 0.0038	- 23.710
H(22)	- 27.990	- 26.364	- 0.9607

**Figure 7.** Cartesian table



**Figure 8.** After Optimization

3. Demethoxycurcumin

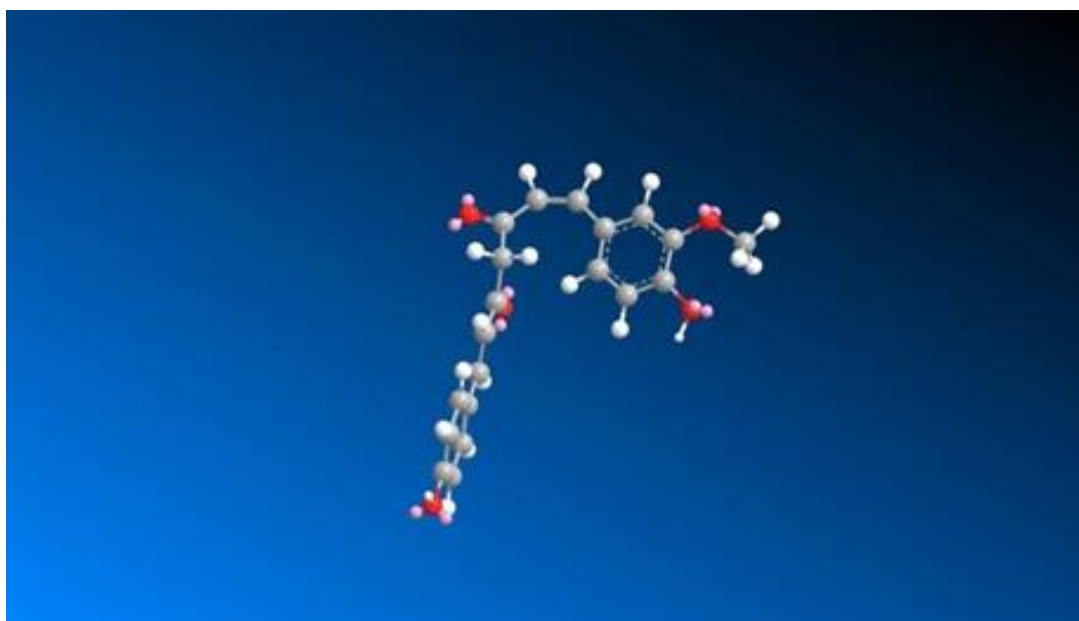


**Figure 9.** Before Optimization



Atom	X (A)	Y(A )	Z(A )
C(1)	26,995	30,113	- 0.8012
C(2)	17,065	21,458	- 0.5720
C(3)	0.4213	25,478	- 0.6811
C(4)	- 0.6994	15.710	- 0.4225
C(5)	- 0.1209	0.2245	- 0.0627
C(6)	- 0.9426	- 0.8121	0.2122
C(7)	- 0.4301	- 20.051	0.5310
O(8)	0.1694	36.893	- 0.9857
O(9)	10.769	0.0734	- 0.0207
C(10)	- 12.433	- 30.309	0.8031
C(11)	- 0.7086	- 42.755	11.356
C(12)	- 15.570	- 53,457	14,194

**Figure 10.** Cartesian Table



**Figure 11.** After Optimization

#### 4.2 Discussion

Based on the data analysis, the research that has been done can be said to be successful. Curcumin is a phytopharmaceutical compound that has several biological effects, namely antidiabetic, antioxidant, anti-inflammatory, antiviral, antifungal effects, inhibits the formation of atherosclerotic plaques, inhibits the growth of *Helicobacter pylori* bacteria, binds mercury and cadmium, prevents cancer, and protects the liver.

Curcumin acts as a strong cancer inhibitor by inhibiting nuclear factor-kappa B and also interferes with the production of harmful and inflammatory glycation end products and leads to cancer mutations in the body. Curcumin effectively inhibits lens epithelial B3 cell proliferation in humans induced by rhbFGF. Curcumin was found to reduce the spread of breast cancer in mice and prevent various forms of cancer. Apart from curcumin, demethoxycurcumin can also be used to prevent cancer, one of which is breast cancer.

## 5. CONCLUSION

Based on descriptive results and data analysis on temulawak, 4 active compounds were obtained, namely curcumin, D-champor, Desmethoxycurcumin and Desmethoxycurcumin. Where in curcumin contains 20% oxidoreductase, 6.7% membrane receptor, 6.7% writer, 20% enzyme and 6.7% protease. Meanwhile, D-champor contains 23.3% nuclear receptor, 20% oxidoreductase, 20% enzyme, 6.7% protease, and 13.3% secreted protein. And Desmethoxycurcumin contains 20% oxidoreductase, 20% enzyme, 6.7% protease and 6.7% membrane receptor. Compounds that act as cancer prevention are curcumin and demethoxycurcumin.

## ACKNOWLEDGEMENTS

Authors may acknowledge to any person, institution or department that supported to any part of study.

## REFERENCES

- [1] Prawati, DD (2019). Factors that influence the incidence of diarrhea in Tambak Sari, Surabaya. *Journal of Health Promotion: The Indonesian Journal of Health Promotion and Health Education* , 7 (1), 34-45.
- [2] Wantoro, A. (2020, October). Application of Fuzzy Logic and Profile Matching in Information Technology of Antibiotic Compatibility Based on Children's Acute Diarrhea. In *SENASTER" National Seminar on Applied Technology Research"* (Vol. 1, No. 1).
- [3] Lima, AA, Oliveira, DB, Quetz, JS, Havt, A., Prata, MM, Lima, I. F. , ... & Guerrant, RL (2019). Etiology and severity of diarrheal diseases in infants at the semiarid region of Brazil: a case-control study. *PLoS neglected tropical diseases* , 13 (2), e0007154.
- [4] Workie, HM, Sharifabdilahi, AS, & Addis, EM (2018). Mothers' knowledge, attitude and practice towards the prevention and home-based management of diarrheal disease among under-five children in Diredawa, Eastern Ethiopia, 2016: a cross-sectional study. *BMC pediatrics* , 18 (1), 1-9.
- [5] Hutasoit, M., Susilowati, L., & Hapzah, IAN (2019). The relationship between mother's knowledge about diarrhea management and diarrhea classification at the Kasihan Bantul Public Health Center. *Medika Respati: Scientific Journal of Health* , 14 (3), 265-276.
- [6] Puspanthani, ME (2019). Analysis of Food Processing by Mothers Based on the Classification of Diarrhea in Early Childhood (1-3 Years) in the Work Area of the Klagenan Public Health Center, Cirebon Regency in 2017. *Syntax Literate; Indonesian Scientific Journal* , 4 (7), 62-74.
- [7] Rizki, VD, & Setyawan, Y. (2018). THE APPLICATION OF THE QUICK, UNBIASED, EFFICIENT —STATISTICAL TREES (QUEST) METHOD TO DETERMINE FACTORS AFFECTING DIARRIC  
<https://journals.insparagonsociety.org/index.php/epicentrum>

- DISEASES IN TODdlERS IN INDONESIA. *Journal of Industrial and Computational Statistics* , 3 (01), 1-10.
- [8] Sy, H., & Syam, A. (2019, August). Data Mining Using the K-Means Algorithm for Grouping the Distribution of Diarrhea in Makassar City. In *SISITI: Scientific Seminar on Information Systems and Information Technology* (Vol. 8, No. 1).
- [9] Harsismanto, J., Oktavidiati, E., & Astuti, D. (2019). The effect of health education on video and poster media on children's knowledge and attitudes in preventing diarrheal diseases. *Journal of Public Health Asclepius* , 1 (1), 75-85.
- [10] Trianto, J. (2018). The application of the forward chaining method for diagnosing diarrheal diseases in children aged 3-5 years based on android mobile. *Journal of Informatics Pamulang University* , 3 (2), 98-103.
- [11] Sumolang, PP, Nurjana, MA, & Widjaja, J. (2019). Analysis of Drinking Water and Hygienic Behavior with the Incidence of Diarrhea in the Elderly in Indonesia. *Health Research and Development Media* , 29 (1), 99-106.
- [12] Juhariyah, S., & Mulyana, SASF (2018). The Relationship between Nutritional Status and the Incidence of Diarrhea in Toddlers at the Rangkasbitung Health Center. *Journal of Obstetrics Scienta* , 6 (1), 219-230.
- [13] Utaminingsyah, F., Siregar, N., & Pohan, SY (2021). The Relationship of Mother's Knowledge and Attitude with Diarrhea in Toddlers in the Children's Room of Padangsidempuan City Hospital in 2020. *Indonesian Health Scientific Journal* , 6 (2), 180-186.
- [14] Apriyanti, RV, Ratnawati, IGA, & Kawuri, R. (2021). THE EFFECT OF ULTRAVIOLET LIGHT ON THE GROWTH OF Enterotoxigenic E. coli (ETEC) bacteria that cause diarrhea. *BIOMA: MAKASSAR JOURNAL OF BIOLOGY* , 6 (1), 66-73.
- [15] Prayoga, P., Muhsinin, S., & Marliani, L. (2021). CHARACTERIZATION AND UTILIZATION OF ENDOPHYTE BACTERIA FROM THE FAMILIA Zingiberaceae in the PHARMACEUTICAL FIELD. *JOPS (Journal Of Pharmacy and Science)* , 4 (2), 51-60.
- [16] Retnaningsih, A. (2019). Inhibitory Test of Turmeric (*Curcuma domestica* Val) and Temulawak (*Curcuma xanthorrhiza* roxb) rhizomes against *Salmonella typhi* bacteria. *Holistic Journal of Health* , 9 (3).
- [17] Novianti, D., & Kartika, T. (2018). MINIMUM INSTRUCTION CONCENTRATION OF BIOACTIVE FRACTION OF TEMULAWAK Rhizome AGAINST *Candida albicans*. *Journal of Biota* , 4 (2), 73-78.
- [18] Zahrah, H., Mustika, A., & Debora, K. (2018). Antibacterial activity and morphological changes of *Propionibacterium acnes* after administration of curcuma xanthorrhiza extract. *Postgraduate Journal of Bioscience* , 20 (3), 160-169.
- [19] Hasibuan, SY, Amallia, C., Hutagalung, MH, & Erawati, S. (2021). Comparison of the Effectiveness of Lemongrass Extract with Temulawak in Inhibiting the Growth of *Streptococcus Mutans*. *Scientific Journal of Health Sandi Husada* , 10 (1), 208-213.
- [20] Indriyanti, R., Hasan, F., & Gartika, M. (2019). DIFFERENCE OF *STREptococcus mutans* BIOFILM REDUCTION BETWEEN N-HEXANE AND ethyl acetate FRACTION OF GARLIC EXTRACT SINGLE GARLIC (*Allium sativum* L.). *ODONTO: Dental Journal* , 6 (1), 21-28.
- [21] Sharif, SN, Hashim, N., Isa, IM, Bakar, SA, Saidin, MI, Ahmad, M. S. , ... & Zainul, R. (2021). Chitosan as a coating material in enhancing the controlled release behavior of zinc hydroxide nitrate–sodium dodecylsulphate–bispyribac nanocomposite. *Chemical Papers* , 75 (2), 611-627.
- [22] Anhar, A., Sumarmin, R., & Zainul, R. (2016). Measurement of glycemic index of West Sumatera local rice genotypes for healthy food selection. *Journal of Chemical and Pharmaceutical Research*, 8(8), 1035-1040.
- [23] Rais, N. S. M., Isa, I. M., Hashim, N., Saidin, M. I., Yazid, S. N. A. M., Ahmad, M. S., ... & Mukdasai, S. (2019). Simultaneously Determination of Bisphenol A and Uric Acid by Zinc/Aluminum-layered Double Hydroxide-2-(2, 4dichlorophenoxy) Propionate Paste Electrode. *International Journal of ELECTROCHEMICAL SCIENCE*, 14, 7911-7924.

- 
- [24] Kharisma, V. D., Agatha, A., Ansori, A. N. M., Widyandana, M. H., Rizky, W. C., Dings, T. G. A., ... & Zainul, R. (2022). Herbal combination from *Moringa oleifera* Lam. and *Curcuma longa* L. as SARS-CoV-2 antiviral via dual inhibitor pathway: A viroinformatics approach. *Journal of Pharmacy and Pharmacognosy Research*, 10(1), 138-146.
- [25] Zainul, R. (2016). Isolation and identification of freshwater microalgae potentially as antibacterial from Talago Biru, Koto Baru, West Sumatera. *Der Pharmacia Lettre*, 8(20), 157-165.
- [26] Zainul, R. (2015). Design of photovoltaic cell with copper oxide electrode by using indoor lights. *Research Journal of Pharmaceutical, Biological and Chemical Sciences*, 6(4), 353-361.
- [27] Mawardi, M., Sanjaya, H., & Zainul, R. (2015). Characterization of Napa soil and adsorption of Pb (II) from aqueous solutions using on column method. *Journal of Chemical and Pharmaceutical Research*, 12(7), 905-912.
- [28] Zainul, R. (2016). Effect of Temperature and Particle Motion against the ability of ZnO Semiconductor Photocatalyst in Humic Acid. *Der Pharmacia Lettre*, 15(8), 120-124. Zainul, R. (2016). Effect of Temperature and Particle Motion against the ability of ZnO Semiconductor Photocatalyst in Humic Acid. *Der Pharmacia Lettre*, 15(8), 120-124.
- [29] Yulis, R., Zainul, R., & Mawardi, M. (2019, April). Effect of natrium sulphate concentration on indoor lights photovoltaic performance. In *Journal of Physics: Conference Series* (Vol. 1185, No. 1, p. 012019). IOP Publishing.
- [30] Nurashikin, A. A., Isa, I. M., Hashim, N., Ahmad, M. S., Zainul, R., Siti, N. A. M. Y., ... & Mukdasai, S. (2020). Synergistic Effect of Zinc/Aluminium-Layered Double Hydroxide-Clopyralid Carbon Nanotubes Paste Electrode in the Electrochemical Response of Dopamine, Acetaminophen, and Bisphenol A. *International Journal of Electrochemical Science*, 15(8), 9088-9107.