



STUDY BIOINFORMATICS WHITE TURMERIC (CURCUMA ZEDOARIA) AGAINST BREAST CANCER

Eko Nevriansyah^a, Sindy Afianti^b, Iga Permata Hani^c, Megawati^d, Widia Novita^e, Fitrah Mey Harmi Siregar^f,
Jumasari Siregar^g

^aMagister Programme of Biochemistry, Postgraduate, Universitas De La Salle, Philippines

^bDepartment of Chemistry, Faculty of Mathematics and Natural Science (FMIPA), Universitas Negeri Padang, JL. Prof. Dr. Hamka, Air Tawar Barat, Padang Utara, 25171 Indonesia

^cDepartment of Biology, Faculty of Mathematics and Natural Science, Universitas Andalas, Limau Manis, Kec. Pauh, Kota Padang, Sumatera Barat 25175, Indonesia

^dDepartment of Agribusiness, Faculty of Agriculture, Universitas Andalas, Limau Manis, Kec. Pauh, Kota Padang, Sumatera Barat 25175, Indonesia

^eDepartment of Mathematics, Faculty of Mathematics and Natural Science (FMIPA), Universitas Islam Negeri Imam Bonjol, Jl. Prof. Mahmud Yunus Lubuk Lintah, Anduring, Kec. Kuranji, Kota Padang, Sumatera Barat 25153, Indonesia

^fMagister Programme of Educational Chemistry, Postgraduate, Universitas Negeri Padang, JL. Prof. Dr. Hamka, Air Tawar Barat, Padang Utara, 25171 Indonesia

^gMagister Programme of Educational Chemistry, Postgraduate, Universitas Negeri Medan, JL. William Iskandar Ps. 5 Medan Estate, North Sumatera, 20221 Indonesia

*Corresponding email: fitrahmey04@gmail.com

ABSTRACT

In Indonesia, almost 70% of people with this disease have experienced cancer, which is found in an advanced stage. This cancer occurs because of an unhealthy lifestyle, so that the immune system decreases. Cancer is usually experienced by many women, one of which is breast cancer. This breast cancer arises from the swelling of the woman's breast area or it can be called a tumor. White turmeric (*Curcuma zedoria*) is a traditional medicine in Indonesia. This white turmeric contains 11 active compounds, there are 5 main active compounds, namely 1,8-cineole, curcumin, D-alpha-pinene, D-borneol and D-champene. The methods used are modeling and computation using phytochem, chemdraw ultra 12.0 and chem 3D Pro 12.0, Switzerland. The conclusion from the results of bioinformatic research on white turmeric extract (*curcuma zedoria*.) Can be used as an anti-breast cancer drug.

Key words: White turmeric; breast cancer

1. INTRODUCTION

This research is about the many medicinal properties of herbs that have not been utilized by researchers until now [1,2]. The method used in this study was ethnobotany, which consisted of using herbal medicines used by certain ethnicities, proven by experimental pharmacological activity and continued with the isolation of compounds that had biological activity[3,4,5,6].

One of the herbal remedies that can be used for medicine, namely white turmeric (*curcuma zedori*) is a plant originating from the Himalayas, India and countries scattered in

Asia[7,8,9]. White turmeric is also found in Indonesia which is used as a traditional medicine in various regions, namely Sumatra, West Java, and Central Java, where the altitude reaches 1000 asl. White turmeric is a rhizomatous or herbaceous type of plant which is an annual plant that grows to form grass with a height of approximately 1 meter, its stems are upright and is a rimbang plant (tubers and underground branches)[10,11]. The chemical content of white turmeric is curcumin, demethoxycumin and essential oil containing monoterpenes (1,8-cineole) and other ingredients such as ethyl-pmethoxycinnamate and D-borneol[12,13,14].

Chemical reactions are very important in life[15]. Where chemical reactions can occur in the stomach, eyes, mouth and other organs. Chemical reactions occur in living things, namely humans, animals and plants and the universe. A chemical reaction will produce new products and new properties, chemical reactions can occur spontaneously or not, there are enormous benefits of chemical reactions in our lives[16].

In white turmeric, which can be used as a cancer drug is its extraction[17]. This extract from white turmeric will react with abnormal body cells, thus helping to stabilize problematic cells. It is suspected that white turmeric contains D-borneol which can attach to abnormal body cells, so that problem cells in the body that should develop are stopped due to the activity of D-borneol sticking[18,19].

2. LITERATURE REVIEW

2.1 Bioinformatics tools used in circRNA research

Since 2012, a large number of bioinformatics tools have been developed for circRNA study[20]. Although the functions of circRNA tools are diverse, they can be classified into three main categories that include circRNA identification tools[21]. A few tools such as disease-associated circRNA databases are technically databases but do not contain primary data. We group tools with similar functions together. Tools that primarily recognize circRNAs are classified as circRNA identification tools[22,23]. Databases that provide basic annotation information are classified as circRNA annotation databases. Finally, stand-alone tools or online services are classified as other tools.

2.2 CircRNA identification tools

Prior to identification, RNA library construction and sequencing provide the raw reads needed. Several library preparation methods can be used for RNA sequencing and subsequent circRNA identification[24]. In theory, polyA⁺ selected RNAs should not contain circRNAs. Nonetheless, libraries sequenced from this selection of RNA may still contain a tiny

proportion of circRNA, because selection is not absolutely accurate. Despite this minor imperfection, polyA⁺ selected datasets can be used as negative controls. Another factor in identification is specificity[25]. To improve this aspect of identification, the false-positive rate of back spliced junction (BSJ) reads can be reduced in various ways. For example, BSJ reads can be supported by its presence in different samples, by a strict cut-off for read counts or by determining whether the circRNA enrichment step is adopted in the library preparation[26]. Most identification tools prefer a circRNA-enriched RNA-Seq dataset as an input. Another strategy is to use paired-end read sequencing to improve the identification of decoy reads that are typically discarded as alignment artifacts. This can be helpful for filtering out false-positive circRNAs.

Notably, most tools have an essential step termed remapping for discovering BSJ reads. Except for segemehl, k-mer based tools and machine-learning-based tools, all identification tools depend on external aligners, with Bowtie, BWA and STAR as the common choices. Most circRNA identification tools belong to the stand-alone category. Nearly all tools release their source code via GitHub and the most popular program language is Python, with R and Perl also being popular languages and Shell as a common choice for building a pipeline. Most pipelines run under Linux or a UNIX-like system. Some tools need to be compiled from source code and some tools need to be manually installed with the dependency environment. Currently, it is more convenient to install tools in Linux, with many tools supporting easy installation methods, such as Conda (bioconda), Docker,

Python package index (PyPI) and BiocManager (Bioconductor)[27]. Most have well-written documents and tutorials to help users install and run their tools. Although installation can be straightforward, some computer science skills may be needed (e.g. programming, Linux system knowledge) to perform an analysis[28]. Therefore, a well-designed, free, online interface or stand-alone tools with a user-friendly interface is generally required for users without advanced computational training. Based on implementation form, circRNA identification tools can be divided into three categories that include BSJ-based, integrated-based and machine learning-based.

3. EXPERIMENTAL

This study uses a systematic literacy review (SLR) method to review studies, assess and interpret and collect information about sedswa contained in white turmeric (curcuma

zedoria) and its role in helping to cure breast cancer [29, 30]. To determine the content, phytochem, chemdraw ultra 12.0, chem 3D Pro 12.0, AND Swiss were used to construct the structure of the compounds that were already in the previous <https://pubchem.ncbi.nlm.nih.gov/> and determine the parameters (coordinate and cartesian tables) in addition to it is also used <http://swisstargetprediction.ch/> to predict the compound is more active to cure any disease.

4. RESULTS AND DISCUSSION

4.1 Chemical content in White Turmeric (*Curcuma Zedoaria*)

Table 1. Data of White Turmeric (*Curcuma Zedoaria*)

Activity	Chemical	Part	Low PPM	High PPM	StdDev
67	1,8-Cineole	Rhizoma	902.0	1920.0	-0,59
5	Bis-Desmethoxycurcumin	Rhizoma	-	1000.0	-1.0
135	Curcumin	Rhizoma	-	1000.0	-0.98
0	D-Alpha-Pinene	Rhizoma	141.0	300.0	
4	D-Borneol	Rhizoma	141.0	300.0	-1.0
0	D-Camphene	Rhizoma	329.0	700.0	1.0
0	D-Cmohor	Rhizoma	395.0	840.0	-1.05
0	EO	Rhizoma	10000.0	1500	
0	Sequiterpene-Alcohols	Rhizoma	4800.0	9600.0	
0	Sesquiterpenes	Rhizoma	1000.0	2000.000	

(source : courtesy of Sindy Afrianti, *et al.*)

After Optimization

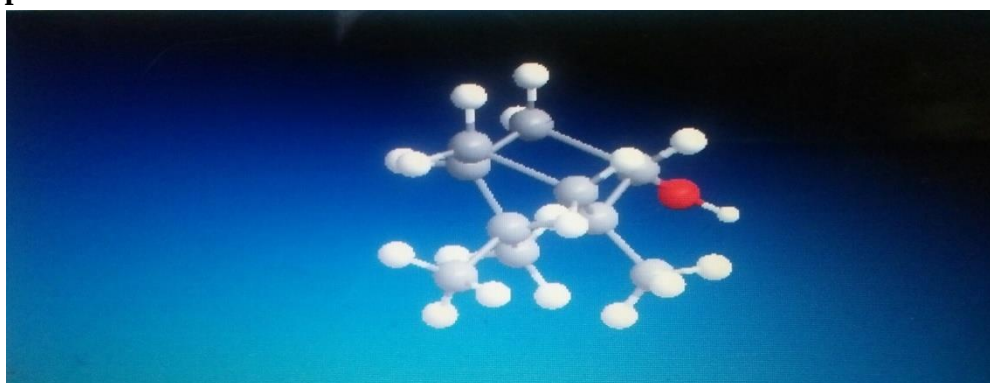


Figure 1. -----MM2-----

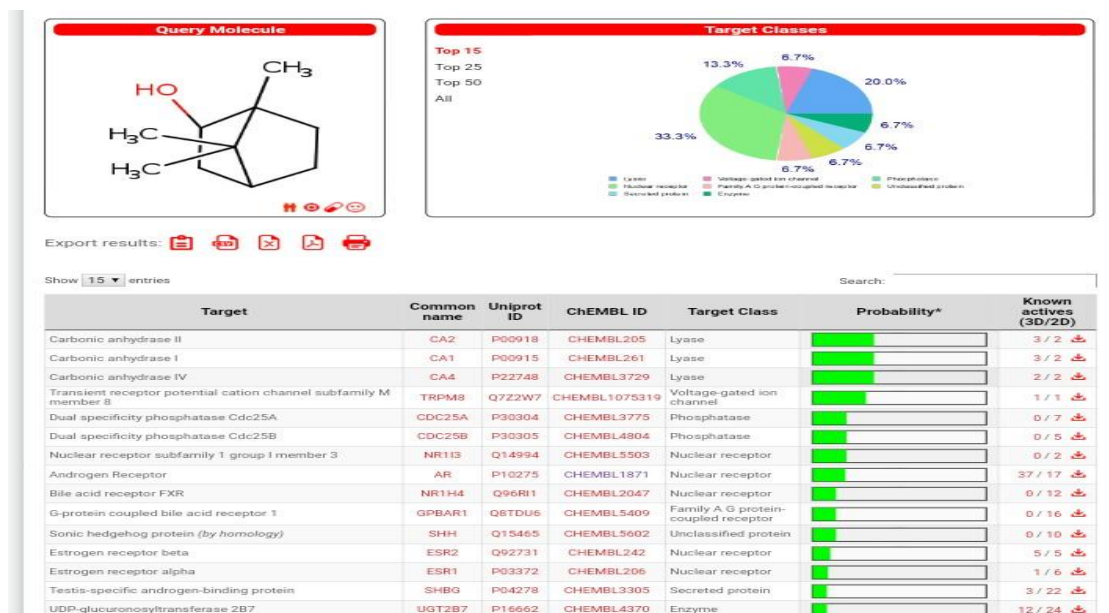
(source : courtesy of Sindy Afrianti, *et al.*)

Table 2. Cartesian Table

Atom	X(A)	Y(A)	Z(A)
C(1)	-0.7961	11.244	0.3227
C(2)	-0.8382	0.6692	-16.222
C(3)	-21.572	-0.0921	-16.222
O(11)	0.3072	0.5598	0.9781
H(12)	-0.7006	22.045	0.5737
H(13)	-0.8728	15.751	-22.678
H(14)	0.0462	0.1222	-20.192

(source : courtesy of Sindy Afrianti, *et al.*)**Table 3. Internal Coordinate Table**

Atom	Atom	Bond	Angle	2nd	2nd	2nd
	Bond	Length	Atom	Angle	atom	angle
						Type
C(1)						
C(2)	C(1)	19.979				
C(3)	C(2)	15.230	C(1)	975.915		
H(13)	C(2)	11.130	C(1)	1.123.277	C(3)	1.123.282 Pro-S
H(14)	C(2)	11.130	C(1)	1.162.630	C(3)	1.162.633 Pro-R
C(4)	C(3)	15.230	C(2)	1.094.700	C(1)	791.358 Dihedral
C(7)	C(3)	15.230	C(2)	1.040.001	C(4)	1.039.999 Pro-R
H(17)	C(4)	11.130	C(3)	1.162.631	C(5)	1.162.629 Pro-S
O(11)	C(1)	14.020	C(2)	1.123.281	C(6)	1.123.281 Pro-S

(source : courtesy of Sindy Afrianti, *et al.*)**Figure 2. target classes**
(source : courtesy of Sindy Afrianti, *et al.*)

5. CONCLUSION

The conclusion from the results of bioinformatic research on white turmeric extract (curcuma zedoria.) Can be used as an anti-breast cancer drug.

ACKNOWLEDGEMENTS

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

REFERENCES

- [1] Zainul, R, Oktavia, B, Nasra, E, Arianti, VA, & ... (2019). Development Study and Effectiveness of Online Data Based Scientific Writing Model Using Endnote Application for MGMP Chemistry Teachers Padang Panjang City. *Pelita* ..., pelitaeksakta.ppj.unp.ac.id, <http://pelitaeksakta.ppj.unp.ac.id/index.php/pelitaeksakta/article/view/43>
- [2] Husna, T, & Zainul, R (2019). The Effect of Acid Bases Learning Media Using Android-Based Chemical Triangle Applications on Learning Outcomes of Class XI High School Students 3 in Padang *International Journal of Progressive Sciences and* ..., ijpsat.es, <http://ijpsat.es/index.php/ijpsat/article/view/949>
- [3] Panmei, R., Gajurel, P. R., & Singh, B. (2019). Ethnobotany of medicinal plants used by the Zeliangrong ethnic group of Manipur, northeast India. *Journal of ethnopharmacology*, 235, 164-182.
- [4] Sarris, J. (2018). Herbal medicines in the treatment of psychiatric disorders: 10-year updated review. *Phytotherapy Research*, 32(7), 1147-1162.
- [5] Nurashikin, AA, Isa, IM, Hashim, N, & ... (2020). Synergistic Effect of Zinc/Aluminium-Layered Double Hydroxide-Clopyralid Carbon Nanotubes Paste Electrode in the Electrochemical Response of Dopamine *International Journal* ..., repository.unp.ac.id, <http://repository.unp.ac.id/35598/>
- [6] Scavone, C., Brusco, S., Bertini, M., Sportiello, L., Rafaniello, C., Zoccoli, A., ... & Capuano, A. (2020). Current pharmacological treatments for COVID-19: What's next?. *British journal of pharmacology*, 177(21), 4813-4824.
- [7] Xu, N., Wang, L., Guan, J., Tang, C., He, N., Zhang, W., & Fu, S. (2018). Wound healing effects of a Curcuma zedoaria polysaccharide with platelet-rich plasma exosomes assembled on chitosan/silk hydrogel sponge in a diabetic rat model. *International journal of biological macromolecules*, 117, 102-107.
- [8] Guney, M., Kumisbek, A., Akimzhanova, Z., Kismelyeva, S., Beisova, K., Zhakiyenova, A., ... & Karaca, F. (2021). Environmental partitioning, spatial distribution, and transport of atmospheric mercury (Hg) originating from a site of former chlor-alkali plant. *Atmosphere*, 12(2), 275.
- [9] MadJin, HM, Hashim, N, Isa, IM, Hussein, MZ, & ... (2020). Synthesis and characterisation of zinc hydroxides nitrates–sodium dodecyl sulphate fluazinam nano hosts for release properties. *Journal of Porous* ..., Springer, <https://doi.org/10.1007/s10934-020-00925-w>
- [10] Pesendorfer, M. B., Bowman, R., Gratzner, G., Pruett, S., Tringali, A., & Fitzpatrick, J. W. (2021). Fire history and weather interact to determine extent and synchrony of mast-seeding in rhizomatous scrub oaks of Florida. *Philosophical Transactions of the Royal Society B*, 376(1839), 20200381.
- [11] Alfarabi, M., & Widyadhari, G. (2018). TOXICITY TEST AND PHYTOCHEMICAL IDENTIFICATION OF RIMBANG (Solanum torvum Swartz) EXTRACT. *AL-KAUNIYAH: Journal of Biology*, 11(2), 109-115.
- [12] Sharif, SNM, Hashim, N, Isa, IM, Bakar, SA, & ... (2020). The impact of a hygroscopic chitosan coating on the controlled release behaviour of zinc hydroxide nitrate–sodium dodecylsulphate–imidacloprid nanocomposites. *New Journal of* ..., pubs.rsc.org, <https://pubs.rsc.org/en/content/articlehtml/2020/nj/d0nj01315c>
- [13] Shafitri, M, & Zainul, R (2019). Vanadium Pentaoksida (V₂O₅): Termodinamika Molecular dan Interaksi Ion dalam Larutan., osf.io, <https://osf.io/preprints/inarxiv/jgmvd/download>
- [14] 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.

- [15] Yazid, SNA Mohd, Isa, I Md, Ali, NM, & ... (2020). Graphene/iridium (III) dimer complex composite modified glassy carbon electrode as selective electrochemical sensor for determination of hydroquinone in real-life *International Journal ...*, Taylor & Francis, <https://doi.org/10.1080/03067319.2020.1758079>
- [16] Ahmad, M. S., Isa, I. M., Hashim, N., Saidin, M. I., Suyanta, S., Zainul, R., ... & Mukdasai, S. (2019). Zinc layered hydroxide-sodium dodecyl sulphate-isopropyl carb modified multiwalled carbon nanotubes as sensor for electrochemical determination of dopamine in alkaline medium. *International Journal of ELECTROCHEMICAL SCIENCE*, 14, 9080-9091. doi: 10.20964/2019.09.54
- [17] Zainul, R., Abd Azis, N., Md Isa, I., Hashim, N., Ahmad, M. S., Saidin, M. I., & Mukdasai, S. (2019). Zinc/aluminium-quinclorac layered nanocomposite modified multi-walled carbon nanotube paste electrode for electrochemical determination of bisphenol A. *Sensors*, 19(4), 941. <https://doi.org/10.3390/s19040941>
- [18] Dong, Z., Zhao, Y., Chen, J., Chang, M., Wang, X., Jin, Q., & Wang, X. (2021). Enzymatic lipophilization of d-borneol extracted from *Cinnamomum camphora* chvar. Borneol seed. *LWT*, 148, 111801.
- [19] Zainul, R., & Wardani, S. W. (2019). The Performance of Hydrogen Generator Based on a 4/4 Al-Cu Plates Designed Sandwich. *Eksakta Berkala Ilmiah Bidang MIPA*, 20(30), 100-104. DOI : 10.24036/eksakta/vol20-iss01/177
- [20] Erhui Xiong, Zhiyong Li, Chen Zhang, Jing Zhang, Ye Liu, Ting Peng, Zhen Chen, Quanzhi Zhao, A study of leaf-senescence genes in rice based on a combination of genomics, proteomics and bioinformatics, *Briefings in Bioinformatics*, Volume 22, Issue 4, July 2021, bbba305, <https://doi.org/10.1093/bib/bbaa305>
- [21] Kharisma, V. D., Ansori, A. N. M., Dian, F. A., Rizky, W. C., Dings, T. G. A., Zainul, R., & Nugraha, A. P. (2021). MOLECULAR DOCKING AND DYNAMIC SIMULATION OF ENTRY INHIBITOR FROM TAMARINDUS INDICA BIOACTIVE COMPOUNDS AGAINST SARS-COV-2 INFECTION VIA VIROINFORMATICS STUDY. *Biochemical and Cellular Archives*, 3323-3327.
- [22] Zainul, R., Oktavia, B., Dewata, I., & Efendi, J. (2018, December). Study of Internal Morphology on Preparation of Cu₂O Thin-Plate using Thermal Oxidation. In *Journal of Physics: Conference Series* (Vol. 1116, No. 4, p. 042046). IOP Publishing. DOI: [10.1088/1742-6596/1116/4/042046](https://doi.org/10.1088/1742-6596/1116/4/042046)
- [23] Wardani, S. W., & Zainul, R. (2019). Efek Variasi Plat Elektroda Cu/Al Pada Generator Hidrogen. *Periodic*, 8(1), 41-45. doi: <https://doi.org/10.24036/p.v8i1.104874>.
- [24] Zainul, R., & Wardani, S. W. (2019). The Performance of Hydrogen Generator Based on a 4/4 Al-Cu Plates Designed Sandwich. *Eksakta Berkala Ilmiah Bidang MIPA*, 20(30), 100-104. DOI : 10.24036/eksakta/vol20-iss01/177
- [25] Zainul, R., Oktavia, B., Dewata, I., & Efendi, J. (2018, April). Thermal and Surface Evaluation on The Process of Forming a Cu₂O/CuO Semiconductor Photocatalyst on a Thin Copper Plate. In *IOP Conference Series: Materials Science and Engineering* (Vol. 335, No. 1, p. 012039). IOP Publishing. DOI: [10.1088/1757-899X/335/1/012039](https://doi.org/10.1088/1757-899X/335/1/012039)
- [26] Nurashikin, A. A., Isa, I. M., Hashim, N., Ahmad, M. S., Siti, N. A. M. Y., Saidin, M. I., ... & Mukdasai, S. (2019). Voltammetric Determination of Bisphenol A in the Presence of Uric Acid Using a Zn/Al-LDH-QM Modified MWCNT Paste Electrode. *International Journal of ELECTROCHEMICAL SCIENCE*, 14. doi: 10.20964/2019.11.46
- [27] Dogu, E., Taheri, S. M., Olivella, R., Marty, F., Lienert, I., Reiter, L., ... & Vitek, O. (2018). MSstatsQC 2.0: R/Bioconductor package for statistical quality control of mass spectrometry-based proteomics experiments. *Journal of proteome research*, 18(2), 678-686.
- [28] Putri, G. E., Arief, S., Jamarun, N., Gusti, F. R., & Zainul, R. (2019). Microstructural analysis and optical properties of nanocrystalline cerium oxides synthesized by precipitation method. *Rasayan J. Chem*, 12(1), 85-90. <http://dx.doi.org/10.31788/RJC.2019.1215029>

-
- [29] Singh, V., & Thurman, A. (2019). How many ways can we define online learning? A systematic literature review of definitions of online learning (1988-2018). *American Journal of Distance Education*, 33(4), 289-306.
- [30] Ferlay, J., Colombet, M., Soerjomataram, I., Parkin, D. M., Piñeros, M., Znaor, A., & Bray, F. (2021). Cancer statistics for the year 2020: An overview. *International Journal of Cancer*, 149(4), 778-789.