

DAFTAR PUSTAKA

- Abu, N., Zamberi, N. R., Yeap, S. K., Nordin, N., Mohamad, N. E., Romli, M. F., Rasol, N. E., Subramani, T., Ismail, N. H., & Alitheen, N. B. 2018. Subchronic toxicity, immunoregulation and anti-breast tumor effect of Nordamnacantal, an anthraquinone extracted from the stems of *Morinda citrifolia* L. *BMC Complementary and Alternative Medicine* 18(1): 1–10. <https://doi.org/10.1186/s12906-018-2102-3>
- Adamson, R. H. 2016. The acute lethal dose 50 (LD50) of caffeine in albino rats. *Regulatory Toxicology and Pharmacology* 80: 274–276. <https://doi.org/10.1016/j.yrtph.2016.07.011>
- Afendi, F. M., Okada, T., Yamazaki, M., Hirai-Morita, A., Nakamura, Y., Nakamura, K., Ikeda, S., Takahashi, H., Altaf-Ul-Amin, M., Darusman, L. K., Saito, K., & Kanaya, S. 2012. KNApSAcK family databases: Integrated metabolite-plant species databases for multifaceted plant research. *Plant and Cell Physiology* 53(2): 1–12. <https://doi.org/10.1093/pcp/pcr165>
- Al-ahmad, M. M., Amir, N., Dhanasekaran, S., John, A., Abdulrazzaq, Y. M., Ali, B. R., & Bastaki, S. M. A. 2017. *Genetic polymorphisms of cytochrome P450- 1A2 (CYP1A2) among Emiratis 2*: 1–13.
- Almeida-Souza, F., De Oliveira, A. E. R., Abreu-Silva, A. L., & Da Silva Calabrese, K. 2018. In vitro activity of *Morinda citrifolia* Linn. fruit juice against the axenic amastigote form of *Leishmania amazonensis* and its hydrogen peroxide induction capacity in BALB/c peritoneal macrophages. *BMC Research Notes* 11(1): 1–7. <https://doi.org/10.1186/s13104-018-3555-7>
- Avdeef, A., Fuguet, E., Llinàs, A., Ràfols, C., Bosch, E., Völgyi, G., Verbic, T., Boldyreva, E., & Takács-Novák, K. 2016. Equilibrium solubility measurement of ionizable drugs - consensus recommendations for improving data quality. *ADMET and DMPK* 4(2): 117–178. <https://doi.org/10.5599/admet.4.2.292>
- Ayob, Z., Mohd Bohari, S. P., Abd Samad, A., & Jamil, S. 2014. Cytotoxic activities against breast cancer cells of local *Justicia gendarussa* crude extracts. *Evidence-Based Complementary and Alternative Medicine* 2014:1-12. <https://doi.org/10.1155/2014/732980>
- Aziz, M. Y. A., Omar, A. R., Subramani, T., Yeap, S. K., Ho, W. Y., Ismail, N. H., Ahmad, S., & Alitheen, N. B. 2014. Damnacanthal is a potent inducer of apoptosis with anticancer activity by stimulating p53 and p21 genes in

- MCF-7 breast cancer cells. *Oncology Letters* 7(5): 1479–1484. <https://doi.org/10.3892/ol.2014.1898>
- Babaji, P., Jagtap, K., Lau, H., Bansal, N., Thajuraj, S., & Sondhi, P. 2016. Comparative evaluation of antimicrobial effect of herbal root canal irrigants (*Morinda citrifolia*, *Azadirachta indica*, *Aloe vera*) with sodium hypochlorite: An in vitro study. *Journal of International Society of Preventive and Community Dentistry* 6(3): 196–199. <https://doi.org/10.4103/2231-0762.183104>
- Baque, M. A., Elgirban, A., Lee, E. J., & Paek, K. Y. 2012. Erratum to: Sucrose regulated enhanced induction of anthraquinone, phenolics, flavonoids biosynthesis and activities of antioxidant enzymes in adventitious root suspension cultures of *Morinda citrifolia* (L.) (*Acta Physiol Plant*, 10.1007/s11738-011-0837-2). *Acta Physiologiae Plantarum* 34(2): 417. <https://doi.org/10.1007/s11738-011-0854-1>
- Beny, R., Yana, N. R. A., & Leorita, M. 2020. Desain Turunan Senyawa Leonurine Sebagai Kandidat Obat Anti Inflamasi. *Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)* 6(1): 181–191. <https://doi.org/10.22487/j24428744.2020.v6.i1.15025>
- Bhal, S. K. 2019. Understanding When to Use Log P & Log D. *ACD/Labs - Advanced Chemistry Development, Inc. Toronto, Canada* 3–6. https://www.acdlabs.com/download/app/physchem/logp_vs_logd.pdf
- Bianchi, F. 2017. Breast cancer: Innovations in research and management. *Breast Cancer: Innovations in Research and Management* 1–928. <https://doi.org/10.1007/978-3-319-48848-6>
- Bleach, R., & McIlroy, M. 2018. The divergent function of androgen receptor in breast cancer; analysis of steroid mediators and tumor intracrinology. *Frontiers in Endocrinology* 9: 1–19. <https://doi.org/10.3389/fendo.2018.00594>
- Bonfield, K., Amato, E., Bankemper, T., Agard, H., Steller, J., Keeler, J. M., Roy, D., McCallum, A., Paula, S., & Ma, L. 2012. Development of a new class of *aromatase* inhibitors: Design, synthesis and inhibitory activity of 3-phenylchroman-4-one (isoflavanone) derivatives. *Bioorganic and Medicinal Chemistry* 20(8): 2603–2613. <https://doi.org/10.1016/j.bmc.2012.02.042>
- Bray, F., Jemal, A., Grey, N., Ferlay, J., & Forman, D. 2012. Global cancer transitions according to the Human Development Index (2008-2030): A population-based study. *The Lancet Oncology* 13(8): 790–801. [https://doi.org/10.1016/S1470-2045\(12\)70211-5](https://doi.org/10.1016/S1470-2045(12)70211-5)

- Budiarsa, I. K., Susilawathi, N. M., Yaputra, F., & Widyadharma, I. P. E. 2019. Sawar Otak. *Callosum Neurology* 2(1): 14–18. <https://doi.org/10.29342/cnj.v2i1.54>
- Bulun, S. E., Lin, Z., Imir, G., Amin, S., Demura, M., Yilmaz, B., Martin, R., Utsunomiya, H., Thung, S., Gurates, B., Tamura, M., Langoi, D., & Deb, S. 2005. Regulation of *aromatase* expression in estrogen-responsive breast and uterine disease: From bench to treatment. *Pharmacological Reviews* 57(3): 359–383. <https://doi.org/10.1124/pr.57.3.6>
- Burley, S. K., Berman, H. M., Bhikadiya, C., Bi, C., Chen, L., Di Costanzo, L., Christie, C., Dalenberg, K., Duarte, J. M., Dutta, S., Feng, Z., Ghosh, S., Goodsell, D. S., Green, R. K., Guranović, V., Guzenko, D., Hudson, B. P., Kalro, T., Liang, Y., ... Zardecki, C. 2019. RCSB Protein Data Bank: Biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. *Nucleic Acids Research* 47(1): 464–D474. <https://doi.org/10.1093/nar/gky1004>
- Buscher, B., Laakso, S., Mascher, H., Pusecker, K., Doig, M., Lieve, D., Wagner-Redeker, W., Pfeifer, T., Pascal, D., & Philip, T. 2014. EBF plasma protein binding. *Bioanalysis* 6(5): 673–682.
- Bussmann, R. W., Hennig, L., Giannis, A., Ortwein, J., Kutchan, T. M., & Feng, X. 2013. Anthraquinone content in noni (*Morinda citrifolia* L.). *Evidence-Based Complementary and Alternative Medicine* 2013: 20–22. <https://doi.org/10.1155/2013/208378>
- Cai, X., Yang, J., Zhou, J., Lu, W., Hu, C., Gu, Z., Huo, J., Wang, X., & Cao, P. 2013. Synthesis and biological evaluation of scopoletin derivatives. *Bioorganic and Medicinal Chemistry* 21(1): 84–92. <https://doi.org/10.1016/j.bmc.2012.10.059>
- Carr, C., Ng, J., & Wigmore, T. 2008. The side effects of chemotherapeutic agents. *Current Anaesthesia and Critical Care* 19(2): 70–79. <https://doi.org/10.1016/j.cacc.2008.01.004>
- Chen, B., McConnell, K. J., Wale, N., Wild, D. J., & Gifford, E. M. 2011. Comparing bioassay response and similarity ensemble approaches to probing protein pharmacology. *Bioinformatics* 27(21): 3044–3049. <https://doi.org/10.1093/bioinformatics/btr506>
- Chumsri, S., Howes, T., Bao, T., Sabnis, G., & Brodie, A. 2011. *Aromatase, aromatase inhibitors, and breast cancer*. *Journal of Steroid Biochemistry and Molecular Biology* 125(2): 13–22. <https://doi.org/10.1016/j.jsbmb.2011>

- Comini, L. R., Fernandez, I. M., Vittar, N. B. R., Núñez Montoya, S. C., Cabrera, J. L., & Rivarola, V. A. 2011. Photodynamic activity of anthraquinones isolated from *Heterophyllaea pustulata* Hook f. (Rubiaceae) on MCF-7c3 breast cancer cells. *Phytomedicine* 18(12): 1093–1095. <https://doi.org/10.1016/j.phymed.2011.05.008>
- Cragg, G. M., & Pezzuto, J. M. 2016. Natural Products as a Vital Source for the Discovery of Cancer Chemotherapeutic and Chemopreventive Agents. *Medical Principles and Practice* 25(2): 41–59. <https://doi.org/10.1159/000443404>
- Dalkas, G. A., Vlachakis, D., Tsagkrasoulis, D., Kastania, A., & Kossida, S. 2013. State-of-the-art technology in modern computer-aided drug design. *Briefings in Bioinformatics* 14(6): 745–752. <https://doi.org/10.1093/bib/bbs063>
- Daly, A. K., Rettie, A. E., Fowler, D. M., & Miners, J. O. 2018. Pharmacogenomics of CYP2C9: Functional and clinical considerations. *Journal of Personalized Medicine* 8(1): 1–31. <https://doi.org/10.3390/jpm8010001>
- Dau, L. 2020. Analisis Molekuler Kandungan Kimia Daun Keladi Tikus (*Typhonium flagelliforme*) dan Daun Sirsak (*Annona muricata*) sebagai Antikanker Payudara dengan Pendekatan Biokemoinformatika. *Skripsi*. Universitas Setia Budi. Surakarta.
- De Los Reyes, M. M., Oyong, G. G., Ng, V. A. S., Shen, C. C., & Ragasa, C. Y. 2017. Cytotoxic compounds from *kibatalia gitingensis* (Elm.) woodson. *Pharmacognosy Journal* 9(1): 8–13. <https://doi.org/10.5530/pj.2017.1.2>
- de Ruyck, J., Brysbaert, G., Blossey, R., & Lensink, M. F. 2016. Molecular docking as a popular tool in drug design, an in silico travel. *Advances and Applications in Bioinformatics and Chemistry* 9(1): 1–11. <https://doi.org/10.2147/AABC.S105289>
- Deng, S., Palu, A. K., West, B. J., Su, C. X., Zhou, B. N., & Jensen, J. C. 2007. Lipoxygenase inhibitory constituents of the fruits of noni (*Morinda citrifolia*) collected in Tahiti. *Journal of Natural Products* 70(5): 859–862. <https://doi.org/10.1021/np0605539>
- Deng, Y., Chin, Y. W., Chai, H., Keller, W. J., & Kinghorn, A. D. 2007. Anthraquinones with quinone reductase-inducing activity and benzophenones from *Morinda citrifolia* (Noni) roots. *Journal of Natural Products* 70(12): 2049–2052. <https://doi.org/10.1021/np070501z>

- Deshmukh, S. R., Habtemariam, S., & Wadegaonkar, P. A. 2010. Antioxidant and antiproliferative activity of root suspension culture of *Morinda citrifolia* L. *Research Journal of Pharmacy and Technology* 3(4): 1189–1193.
- Devi, C. H. K., & Krishna, D. G. 2013. Phytochemical screening, antibacterial, antifungal and anthelmintic activity of *Morinda citrifolia* stem. *Journal of Pharmacognosy and Phytochemistry* 2(1): 115–117.
- Dickson, C. J., Velez-Vega, C., & Duca, J. S. 2020. Revealing Molecular Determinants of hERG Blocker and Activator Binding. *Journal of Chemical Information and Modeling* 60(1): 192–203. <https://doi.org/10.1021/acs.jcim.9b00773>
- Didziapetris, R., Japertas, P., Avdeef, A., & Petrauskas, A. 2003. Classification analysis of P-glycoprotein substrate specificity. *Journal of Drug Targeting* 11(7): 391–406. <https://doi.org/10.1080/10611860310001648248>
- Ding, Y., Nguyen, H. T., Kim, S. I., Kim, H. W., & Kim, Y. H. 2009. The regulation of inflammatory cytokine secretion in macrophage cell line by the chemical constituents of *Rhus sylvestris*. *Bioorganic and Medicinal Chemistry Letters* 19(13): 3607–3610. <https://doi.org/10.1016/j.bmcl.2009.04.129>
- Dixit, B. 2017. A review on the effects of frequency of. *Bioinformatics Review*, 3(9): 1155–1165.
- Doak, B. C., Over, B., Giordanetto, F., & Kihlberg, J. 2014. Oral druggable space beyond the rule of 5: Insights from drugs and clinical candidates. *Chemistry and Biology* 21(9): 1115–1142. <https://doi.org/10.1016/j.chembiol.2014.08.013>.
- Dong, H., Zou, M., Bhatia, A., Jayaprakash, P., Hofman, F., Ying, Q., Chen, M., Woodley, D. T., & Li, W. 2016. Breast Cancer MDA-MB-231 Cells Use Secreted Heat Shock Protein-90alpha (Hsp90 α) to Survive a Hostile Hypoxic Environment. *Scientific Reports* 6(1): 1–9. <https://doi.org/10.1038/srep20605>
- Eom, Y. H., Kim, H. S., Lee, A., Song, B. J., & Chae, B. J. 2016. BCL2 as a subtype-specific prognostic marker for breast cancer. *Journal of Breast Cancer* 19(3): 252–260. <https://doi.org/10.4048/jbc.2016.19.3.252>
- Febriansah Desy; Hardika, Dwi Susilo; Prabaningrum, Dita; Hadi, Dzilqi Bustanul; Oktafiyani, Nur, R. B. 2012. Kajian secara In Vitro Ekstrak Etanolik Buah *Morinda citrifolia* L. sebagai Agen Khemopreventif Kanker Payudara yang Potensial. *Jurnal Mutiara Medika* 12(3): 155–162. <http://journal.umy.ac.id/index.php/mm/article/view/1038>

- Febriansah Desy; Hardika, Dwi Susilo; Prabaningrum, Dita; Hadi, Dzilqi Bustanul; Oktafiyani, Nur, R. B. 2012. Kajian secara In Vitro Ekstrak Etanolik Buah Morinda citrifolia L. sebagai Agen Khemopreventif Kanker Payudara yang Potensial. *Jurnal Mutiara Medika* 12(3): 155–162. <http://journal.umy.ac.id/index.php/mm/article/view/1038>
- Feinberg, E. N., Joshi, E., Pande, V. S., & Cheng, A. C. 2020. Improvement in ADMET Prediction with Multitask Deep Featurization. *Journal of Medicinal Chemistry* 63(16):8835–8848. <https://doi.org/10.1021/acs.jmedchem.9b02187>
- Ferreira, L. G., Dos Santos, R. N., Oliva, G., & Andricopulo, A. D. 2015. Molecular docking and structure-based drug design strategies. *Jurnal Molecules* 20(7). <https://doi.org/10.3390/molecules200713384>
- Finch, A., & Pillans, P. 2014. P-glycoprotein and its role in drug-drug interactions. *Australian Prescriber* 37(4): 137–139. <https://doi.org/10.18773/austprescr.2014.050>
- Föllmann, W., Degen, G., Oesch, F., & Hengstler, J. G. 2013. Ames Test. *Elsevier Inc* 1:104-107. <https://doi.org/10.1016/B978-0-12-374984-0.00048-6>
- Fotia, C., Avnet, S., Granchi, D., & Baldini, N. 2012. The natural compound Alizarin as an osteotropic drug for the treatment of bone tumors. *Journal of Orthopaedic Research* 30(9): 1486–1492. <https://doi.org/10.1002/jor.22101>
- G. Grothaus, P., M. Cragg, G., & J. Newman, D. 2010. Plant Natural Products in Anticancer Drug Discovery. *Current Organic Chemistry* 14(16): 1781–1791. <https://doi.org/10.2174/138527210792927708>
- Garcia-Cortes, M., Robles-Diaz, M., Stephens, C., Ortega-Alonso, A., Lucena, M. I., & Andrade, R. J. 2020. Drug induced liver injury: an update. *Archives of Toxicology* 94(10): 3381–3407. <https://doi.org/10.1007/s00204-020-02885-1>
- Gfeller, D., Grosdidier, A., Wirth, M., Daina, A., Michielin, O., & Zoete, V. 2014. SwissTargetPrediction: A web server for target prediction of bioactive small molecules. *Nucleic Acids Research* 42(1): 32–38. <https://doi.org/10.1093/nar/gku293>
- Ghali, R. M., Al-Mutawa, M. A., Al-Ansari, A. K., Zaied, S., Bhiri, H., Mahjoub, T., & Almawi, W. Y. 2018. Differential association of ESR1 and ESR2 gene variants with the risk of breast cancer and associated features: A case-control study. *Gene* 651: 194–199. <https://doi.org/10.1016/j.gene.2018.02.011>

- Ghosh, D., Griswold, J., Erman, M., & Pangborn, W. 2010. X-ray structure of human *aromatase* reveals an androgen-specific active site. *Journal of Steroid Biochemistry and Molecular Biology* 118(5): 197–202. <https://doi.org/10.1016/j.jsbmb.2009.09.012>
- Girault, I., Bièche, I., & Lidereau, R. 2006. Role of estrogen receptor α transcriptional coregulators in tamoxifen resistance in breast cancer. *Maturitas* 54(4): 342–351. <https://doi.org/10.1016/j.maturitas.2006.06.003>
- Gómez-Lechón, M. J., Tolosa, L., Conde, I., & Donato, M. T. 2014. Competency of different cell models to predict human hepatotoxic drugs. *Expert Opinion on Drug Metabolism and Toxicology* 10(11): 1553–1568. <https://doi.org/10.1517/17425255.2014.967680>
- Hairunnisa, H. 2019. Sulitnya Menemukan Obat Baru di Indonesia. *Majalah Farmasetika*. 4(1): 16.
- Han, B., Jiang, P., Liu, W., Xu, H., Li, Y., Li, Z., Ma, H., Yu, Y., Li, X., & Ye, X. 2018. Role of Daucosterol Linoleate on Breast Cancer: Studies on Apoptosis and Metastasis. *Journal of Agricultural and Food Chemistry* 66(24): 6031–6041. <https://doi.org/10.1021/acs.jafc.8b01387>
- Hanahan, D., & Weinberg, R. A. 2011. Hallmarks of cancer: The next generation. *Cell* 144(5): 646–674. <https://doi.org/10.1016/j.cell.2011.02.013>
- Handayani, D. P. 2015. Uji Kombinasi Ekstrak Etil Asetat Buah Mengkudu (*Morinda citrifolia* L.) dengan Senyawa Doxorubicin pada Sel Kanker Payudara MCF-7 Secara In Vitro dan In Silico. *Karya Tulis Ilmiah*. Universitas Muhammadiyah Yogyakarta. Yogyakarta.
- Harahap, U., Haro, G., Purnomo, H., & Satria, D. 2020. In Silico Analysis of Boron Derivate Compounds as Potential ER- α Inhibitor. *Icosteerr* 814–817. <https://doi.org/10.5220/0010091808140817>
- Harris, R. E., Casto, B. C., & Harris, Z. M. 2014. Cyclooxygenase-2 and the inflammogenesis of breast cancer. *World Journal of Clinical Oncology* 5(4): 677–692. <https://doi.org/10.5306/wjco.v5.i4.677>
- Haryanti, S., & Widiyastuti, Y. 2017. Aktivitas Sitotoksik pada Sel MCF-7 dari Tumbuhan Indonesia untuk Pengobatan Tradisional Kanker Payudara. *Media Penelitian Dan Pengembangan Kesehatan* 27(4): 247–254. <https://doi.org/10.22435/mpk.v27i4.5010.247-254>
- Hasanah, A. N., & Rusdiana, T. 2018. METODE PENAMBAHAN SURFAKTAN SEBAGAI SUBSTRAT PG-P UNTUK

MENINGKATKAN KELARUTAN OBAT LIPOFILIK : ARTICLE REVIEW Amira. *Farmaka*. 16(2): 42–50.

- Hedley, P. L., Jørgensen, P., Schlamowitz, S., Wangari, R., Moolman-Smook, J., Brink, P. A., Kanters, J. K., Corfield, V. A., & Christiansen, M. 2009. The genetic basis of long QT and short QT syndromes: A mutation update. *Human Mutation* 30(11): 1486–1511. <https://doi.org/10.1002/humu.21106>
- Herdwiani, W. 2020. *Biofarmasetika Dan Farmakokinetika*. Trans Info Media.
- Hodaei, D., Baradaran, B., Valizadeh, H., & Zakeri-Milani, P. 2015. Effects of polyethylene glycols on intestinal efflux pump expression and activity in Caco-2 cells. *Brazilian Journal of Pharmaceutical Sciences* 51(3): 745–754. <https://doi.org/10.1590/S1984-82502015000300026>
- Horde, G., & Gupta, V. 2021. *Drug Clearance*. StatPearls Publishing, Treasure Island (FL).
- Hospital Authority. 2021. Breast Cancer. <https://www21.ha.org.hk/smartpatient/SPW/en-us/Disease-Information/Disease/?guid=bc5c075d-d161-4abc-9b1b-1b1ca15d6947>. 16 Maret 2021 (16:38).
- Hubatsch, I., Ragnarsson, E. G. E., & Artursson, P. 2007. Determination of drug permeability and prediction of drug absorption in Caco-2 monolayers. *Nature Protocols* 2(9): 2111–2119. <https://doi.org/10.1038/nprot.2007.303>
- Huff, H. C., Vasan, A., Roy, P., Kaul, A., Tajkhorshid, E., & Das, A. 2021. Differential Interactions of Selected Phytocannabinoids with Human CYP2D6 Polymorphisms. *Biochemistry* 60(37): 2749–2760. <https://doi.org/10.1021/acs.biochem.1c00158>
- Huss, L., Butt, S. T., Borgquist, S., Elebro, K., Sandsveden, M., Rosendahl, A., & Manjer, J. 2019. Vitamin D receptor expression in invasive breast tumors and breast cancer survival. *Breast Cancer Research* 21(1): 1–13. <https://doi.org/10.1186/s13058-019-1169-1>
- ITIS. 2021. *Morinda citrifolia* L. ITIS Report. https://www.itis.gov/servlet/SingleRpt/SingleRpt?search_topic=TSN&search_value=35071#null. 3 Maret 2021 (17:30).
- Jamkhande, P. G., Ghante, M. H., & Ajgunde, B. R. 2017. Software based approaches for drug designing and development: A systematic review on commonly used software and its applications. *Bulletin of Faculty of Pharmacy, Cairo University* 55(2): 203–210. <https://doi.org/10.1016/j.bfopcu.2017.10.001>

- Joo, W. D., Visintin, I., & Mor, G. 2013. Targeted cancer therapy - Are the days of systemic chemotherapy numbered? *Maturitas* 76(4): 308–314. <https://doi.org/10.1016/j.maturitas.2013.09.008>
- Kamiya, K., Hamabe, W., Tokuyama, S., Hirano, K., Satake, T., Kumamoto-Yonezawa, Y., Yoshida, H., & Mizushima, Y. 2010. Inhibitory effect of anthraquinones isolated from the Noni (*Morinda citrifolia*) root on animal A-, B- and Y-families of DNA polymerases and human cancer cell proliferation. *Food Chemistry* 118(3): 725–730. <https://doi.org/10.1016/j.foodchem.2009.05.053>
- Kapelyukh, Y., Henderson, C. J., Scheer, N., Rode, A., & Wolf, C. R. 2019. Defining the contribution of CYP1A1 and CYP1A2 to drug metabolism using humanized CYP1A1/1A2 and Cyp1a1/Cyp1a2 knockout mice. *Drug Metabolism and Disposition* 47(8): 907–918. <https://doi.org/10.1124/dmd.119.087718>
- Kilo, A. La, Aman, L. O., Sabihi, I., & Kilo, J. La. 2019. Studi Potensi Pirazolin Tersubstitusi 1-N Dari Tiosemikarbazon Sebagai Agen Antiamuba Melalui Uji In Silico 7(1): 1–23
- Kilo, A. La, Aman, L. O., Sabihi, I., & Kilo, J. La. 2019. Studi Potensi Pirazolin Tersubstitusi 1-N Dari Tiosemikarbazon Sebagai Agen Antiamuba Melalui Uji In Silico 7(1): 1–23
- Kim, M. T., Sedykh, A., Chakravarti, S. K., Saiakhov, R. D., & Zhu, H. 2014. Critical evaluation of human oral bioavailability for pharmaceutical drugs by using various cheminformatics approaches. *Pharmaceutical Research* 31(4): 1002–1014. <https://doi.org/10.1007/s11095-013-1222-1>
- Kim, S., Thiessen, P. A., Bolton, E. E., Chen, J., Fu, G., Gindulyte, A., Han, L., He, J., He, S., Shoemaker, B. A., Wang, J., Yu, B., Zhang, J., & Bryant, S. H. 2016. PubChem substance and compound databases. *Nucleic Acids Research* 44(1): 1202–1213. <https://doi.org/10.1093/nar/gkv951>
- Kong, Q., Ma, Y., Yu, J., & Chen, X. 2017. Predicted molecular targets and pathways for germacrone, curdione, and furanodiene in the treatment of breast cancer using a bioinformatics approach. *Scientific Reports* 7(1): 1–11. <https://doi.org/10.1038/s41598-017-15812-9>
- Korb, O. 2009. Efficient ant colony optimization algorithms for structure- and ligand-based drug design. *Chemistry Central Journal* 3(1): 4150. <https://doi.org/10.1186/1752-153X-3-S1-O10>
- Kramer, S. D., Aschmann, H. E., Hatibovic, M., Hermann, K. F., Neuhaus, C. S., Brunner, C., & Belli, S. 2016. When barriers ignore the “rule-of-five.”

Advanced Drug Delivery Reviews 101: 62–74.
<https://doi.org/10.1016/j.addr.2016.02.001>

- Kumar, R., Sharma, A., Siddiqui, M. H., & Tiwari, R. K. 2017. Prediction of Drug-Plasma Protein Binding Using Artificial Intelligence Based Algorithms. *Combinatorial Chemistry & High Throughput Screening* 21(1): 57–64. <https://doi.org/10.2174/1386207321666171218121557>
- Land, H., & Humble, M. S. 2018. YASARA: A tool to obtain structural guidance in biocatalytic investigations. *Methods in Molecular Biology* 1685: 43–67. https://doi.org/10.1007/978-1-4939-7366-8_4
- Latif, M. S., Rusdiana, T., & Gozali, D. 2018. Pengaruh P-Glycoprotein (P-GP) Terhadap Bioavailabilitas Atorvastatin. *HMG-CoA Reductase Inhibitors and P-Glycoprotein Modulation* 16: 1183–1192.
- Latif, M., Ashraf, Z., Basit, S., Ghaffar, A., Zafar, M. S., Saeed, A., & Meo, S. A. 2018. Latest perspectives of orally bioavailable 2,4-diarylaminopyrimidine analogues (DAAPalogues) as anaplastic lymphoma kinase inhibitors: discovery and clinical developments. *RSC Advances* 8(30): 16470–16493. <https://doi.org/10.1039/c8ra01934g>
- Lee, K. H., Koh, M., & Moon, A. 2016. Farnesyl transferase inhibitor FTI-277 inhibits breast cell invasion and migration by blocking H-Ras activation. *Oncology Letters* 12(3): 2222–2226. <https://doi.org/10.3892/ol.2016.4837>
- Liao, X. H., Lu, D. L., Wang, N., Liu, L. Y., Wang, Y., Li, Y. Q., Yan, T. B., Sun, X. G., Hu, P., & Zhang, T. C. 2014. Estrogen receptor α mediates proliferation of breast cancer MCF-7 cells via a p21/PCNA/E2F1-dependent pathway. *FEBS Journal* 281(3): 927–942. <https://doi.org/10.1111/febs.12658>
- Lim, S. L., Goh, Y. M., Noordin, M. M., Rahman, H. S., Othman, H. H., Abu Bakar, N. A., & Mohamed, S. 2016. Morinda citrifolia edible leaf extract enhanced immune response against lung cancer. *Food and Function* 7(2): 741–751. <https://doi.org/10.1039/c5fo01475a>
- Lim, S. L., Mustapha, N. M., Goh, Y. M., Bakar, N. A. A., & Mohamed, S. 2016. Metastasized lung cancer suppression by Morinda citrifolia (Noni) leaf compared to Erlotinib via anti-inflammatory, endogenous antioxidant responses and apoptotic gene activation. *Molecular and Cellular Biochemistry* 416(1–2): 85–97. <https://doi.org/10.1007/s11010-016-2698-x>
- Listyani, T. A., Herowati, R., & Djalil, A. D. 2019. Analisis Docking Molekuler Senyawa Derivat Phthalimide sebagai Inhibitor Non-Nukleosida HIV-1

- Reverse Transcriptase. *Jurnal Farmasi Indonesia* 15(2): 123–134. <https://doi.org/10.31001/jfi.v15i2.445>
- LIU, C. hong, XUE, Y. rong, YE, Y. hang, YUAN, F. feng, LIU, J. yan, & SHUANG, J. lei. 2007. Extraction and Characterization of Antioxidant Compositions From Fermented Fruit Juice of *Morinda citrifolia* (Noni). *Agricultural Sciences in China* 6(12): 1494–1501. [https://doi.org/10.1016/S1671-2927\(08\)60013-9](https://doi.org/10.1016/S1671-2927(08)60013-9)
- López-Biedma, A., Sánchez-Quesada, C., Beltrán, G., Delgado-Rodríguez, M., & Gaforio, J. J. 2016. Phytoestrogen (+)-pinoresinol exerts antitumor activity in breast cancer cells with different oestrogen receptor statuses. *BMC Complementary and Alternative Medicine* 16(1): 1–14. <https://doi.org/10.1186/s12906-016-1233-7>
- LoRusso, P. M. 2012. Mammalian target of rapamycin as a rational therapeutic target for breast cancer treatment. *Oncology (Switzerland)* 84(1): 43–56. <https://doi.org/10.1159/000343063>
- Lv, L., Chen, H., Ho, C. T., & Sang, S. 2011. Chemical components of the roots of Noni (*Morinda citrifolia*) and their cytotoxic effects. *Fitoterapia* 82(4): 704–708. <https://doi.org/10.1016/j.fitote.2011.02.008>
- Macalino, S. J. Y., Gosu, V., Hong, S., & Choi, S. 2015. Role of computer-aided drug design in modern drug discovery. *Archives of Pharmacal Research* 38(9): 1686–1701. <https://doi.org/10.1007/s12272-015-0640-5>
- Maennling, A. E., Tur, M. K., Niebert, M., Klockenbring, T., Zeppernick, F., Gattenlöhner, S., Meinhold-Heerlein, I., & Hussain, A. F. 2019. Molecular targeting therapy against egfr family in breast cancer: Progress and future potentials. *Cancers* 11(12): 1–19. <https://doi.org/10.3390/cancers11121826>
- Martin, L. A., & Dowsett, M. 2013. BCL-2: A New Therapeutic Target in Estrogen Receptor-Positive Breast Cancer? *Cancer Cell* 24(1): 7–9. <https://doi.org/10.1016/j.ccr.2013.06.006>
- Meli, M., Shafie, N., Loh, S., & Rahmat, A. 2019. Anti-proliferative and apoptosis-inducing effects of *Morinda citrifolia* L. shoot on breast, liver, and colorectal cancer cell lines. *Malaysian Journal of Medicine and Health Sciences* 15(1): 129–135.
- Mittal, B., Tulsyan, S., Kumar, S., Mittal, R. D., & Agarwal, G. 2015. Cytochrome P450 in Cancer Susceptibility and Treatment. *Elsevier Inc* 71. <https://doi.org/10.1016/bs.acc.2015.06.003>

- Mo, S.-L., Zhou, Z.-W., Yang, L.-P., Wei, M., & Zhou, S.-F. 2010. New Insights into the Structural Features and Functional Relevance of Human Cytochrome P450 2C9. Part I. *Current Drug Metabolism* 10(10): 1075–1126. <https://doi.org/10.2174/138920009790820129>
- Monika, G., Punam, G., Sarbjot, S., & G.D., G. 2010. An Overview ON Molecular Docking. *International Journal of Drug Development & Research* 2(2): 219.
- Morris, G. M., & Lim-Wilby, M. 2008. Molecular Docking. *Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine* 443: 1149–1153. https://doi.org/10.1007/3-540-29623-9_3820
- Muchtaridi, M., Syahidah, H. N., Subarnas, A., Yusuf, M., Bryant, S. D., & Langer, T. 2017. Molecular docking and 3D-pharmacophore modeling to study the interactions of chalcone derivatives with estrogen receptor alpha. *Pharmaceuticals* 10(4): 1–12. <https://doi.org/10.3390/ph10040081>
- Mulders, M., Vingerhoets, A., & Breed, W. 2008. The impact of cancer and chemotherapy: Perceptual similarities and differences between cancer patients, nurses and physicians. *European Journal of Oncology Nursing* 12(2): 97–102. <https://doi.org/10.1016/j.ejon.2007.10.002>
- Murakami, T. 2017. Absorption sites of orally administered drugs in the small intestine. *Expert Opinion on Drug Discovery* 12(12): 1219–1232. <https://doi.org/10.1080/17460441.2017.1378176>
- Murray, A., Madden, S. F., Synnott, N., Klinger, R., O’Connot, D., O’Donovan, N., Gallagher, W., Crown, J., & Duffy, M. J. 2013. *Vitamin D Receptor as a Target for Breast Cancer Therapy* 1986(412): 1–42. <https://doi.org/https://doi.org/10.1530/ERC-16-0463>
- National Center for Biotechnology Information. 2021. PubChem Bioassay Record for AID 1195, Source: EPA DSSTox. Retrieved November 3, 2021 from <https://pubchem.ncbi.nlm.nih.gov/bioassay/1195>.
- Neal, M. J. 2016. Medical pharmacology at a glance. In *Progress in Medicinal Chemistry*. 8th ed. John Wiley & Sons. Singapore. [https://doi.org/10.1016/S0079-6468\(08\)70167-X](https://doi.org/10.1016/S0079-6468(08)70167-X)
- Nelson, S. C. 2003. *Morinda citrifolia*. *Edible Medicinal And Non-Medicinal Plants* 715–753. https://doi.org/10.1007/978-94-007-5653-3_35
- Obermann, W. M. J. 2018. A motif in HSP90 and P23 that links molecular chaperones to efficient estrogen receptor α methylation by the lysine

- methyltransferase SMYD2. *Journal of Biological Chemistry* 293(42): 16479–16487. <https://doi.org/10.1074/jbc.RA118.003578>
- Pandi, P., Selvam, & Guptha, R. M. 2015. *Lc-Ms / Ms Studies on the Fruit Extracts of Morinda* 4(9), 2281–2298
- Parveen, I., Ahmed, N., Idrees, D., Khan, P., & Hassan, M. I. 2017. Synthesis, estrogen receptor binding affinity and molecular docking of pyrimidine-piperazine-chromene and -quinoline conjugates. *Bioorganic and Medicinal Chemistry Letters* 27(18): 4493–4499. <https://doi.org/10.1016/j.bmcl.2017.07.077>
- Patrick, G. L. 2013. Introduction to medicinal chemistry. In *Oxford*. [https://doi.org/10.1016/0307-4412\(76\)90096-0](https://doi.org/10.1016/0307-4412(76)90096-0)
- Paudel, A., Panthee, S., Urai, M., Hamamoto, H., Ohwada, T., & Sekimizu, K. 2018. Pharmacokinetic parameters explain the therapeutic activity of antimicrobial agents in a silkworm infection model. *Scientific Reports* 8(1): 1–8. <https://doi.org/10.1038/s41598-018-19867-0>
- Paul, A. 2019. *Drug Distribution*. Springer International Publishing. https://doi.org/https://doi.org/10.1007/978-981-32-9779-1_6
- Pedretti, A., Mazzolari, A., Vistoli, G., Farmaceutica, C., Pratesi, P., & Farmacia, F. 2004. VEGA ZZ: a versatile toolkit for drug design and protein modelling. *J Comput Chem* 21(2002): 20133.
- Pertiwi, Y. U. P., Prajitno, A., & Fadjar, M. 2019. Analysis of Metabolit and Antibacterial Control of Mengkudu Leaf Extract (*Morinda citrifolia*) on the Bacteria of *Aeromonas hydrophila*. *Research Journal of Life Science* 6(3): 172–183. <https://doi.org/10.21776/ub.rjls.2019.006.03.3>
- Petrović, J., Pešić, V., & Lauschke, V. M. 2020. Frequencies of clinically important CYP2C19 and CYP2D6 alleles are graded across Europe. *European Journal of Human Genetics* 28(1): 88–94. <https://doi.org/10.1038/s41431-019-0480-8>
- Piaz, F. D., Terracciano, S., De Tommasi, N., & Braca, A. 2015. Hsp90 Activity Modulation by Plant Secondary Metabolites. *Planta Medica* 81(14): 1223–1239. <https://doi.org/10.1055/s-0035-1546251>
- Pranowo, H. D. 2004. *Kimia Komputasi*. Austrian-Indonesian Centre for Computational Chemistry (AIC).
- Pratama, M. R. F., Poerwono, H., & Siswodihardjo, S. 2020. Molecular docking of novel 5-O-benzoylpinostrobin derivatives as SARS-CoV-2 main

- protease inhibitors. *Pharmaceutical Sciences* 26(1): 63–77. <https://doi.org/10.34172/PS.2020.57>
- Pratiwi, D., Insanu, M., & Damayanti, S. 2014. *Prediksi Toksisitas Senyawa Antioksidan Alami dan Analisis Interaksinya Terhadap Reseptor VEGF-1 Menggunakan Metode Molecular Docking* 1(1): 1–9.
- Purnomo, H. 2013. *Kimia Komputasi untuk Farmasi dan Ilmu Terkait Uji in Siliko Senyawa Antikanker*. 1st ed. Pustaka Pelajar. Yogyakarta.
- Puspaningtyas, A. R. 2012. Molekular Docking Dengan Metode Molegro Virtual Docker Turunan Kalkon Sebagai Antimikroba. *Stomatognatic (J.K.G Unej)* 9(1): 39–47.
- Rahayu, M., & Solihat, M. F. 2018. *Toksikologi Klinik*. Kementerian Kesehatan RI.
- Ramli, M. 2015. Update Breast Cancer Management. *Jurnal Fakultas Kedokteran Andalas* 38: 28–52.
- Rana, J., & Vaisla, K. S. 2013. Introduction to bioinformatics. *Functional Plant Genomics* 53–55. <https://doi.org/10.1201/b13091-1>
- Ricart, A. D. 2017. Drug-induced liver injury in Oncology. *Annals of Oncology*, 28(8), 2013–2020. <https://doi.org/10.1093/annonc/mdx158>
- Rose, P. W., Prlić, A., Altunkaya, A., Bi, C., Bradley, A. R., Christie, C. H., Di Costanzo, L., Duarte, J. M., Dutta, S., Feng, Z., Green, R. K., Goodsell, D. S., Hudson, B., Kalro, T., Lowe, R., Peisach, E., Randle, C., Rose, A. S., Shao, C., ... Burley, S. K. 2017. The RCSB protein data bank: Integrative view of protein, gene and 3D structural information. *Nucleic Acids Research* 45(1): 271–281. <https://doi.org/10.1093/nar/gkw1000>
- Rosenbaum, S. E. 2016. *Basic Pharmacokinetics and Pharmacodynamics: An Integrated Textbook and Computer Simulations* (2nd ed.). Wiley.
- Roy, P. P., & Roy, K. 2010. Molecular docking and QSAR studies of aromatase inhibitor androstenedione derivatives. *Journal of Pharmacy and Pharmacology* 62(12): 1717–1728. <https://doi.org/10.1111/j.2042-7158.2010.01154.x>
- Rubin, E., & Reisner, H. M. 2013. Rubin's Pathology Six Edition. In *Journal of Chemical Information and Modeling*. 6th ed. Lippincott Williams & Wilkins. Philadelphia.

- Ruff, M., Gangloff, M., Marie Wurtz, J., & Moras, D. 2000. Estrogen receptor transcription and transactivation Structure-function relationship in DNA- and ligand-binding domains of estrogen receptors. *Breast Cancer Research* 2(5). <https://doi.org/10.1186/bcr80>
- Ruslin, Yana, N. R. A., & Leorita, M. 2020. Desain Turunan Senyawa Leonurine Sebagai Kandidat Obat Anti Inflamasi. *Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)* 6(1): 181–191. <https://doi.org/10.22487/j24428744.2020.v6.i1.15025>
- Saha, K., Lam, K. W., Abas, F., Sazali Hamzah, A., Stanslas, J., Hui, L. S., & Lajis, N. H. 2013. Synthesis of damnacanthal, a naturally occurring 9,10-anthraquinone and its analogues, and its biological evaluation against five cancer cell lines. *Medicinal Chemistry Research* 22(5): 2093–2104. <https://doi.org/10.1007/s00044-012-0197-5>
- Sari, I. K., Arisandi, M., Morika, H. D., & Novrika, B. 2018. Pengaruh Pemberian Air Perasan Buah Mengkudu (Morinda Citrifolia) Terhadap Penurunan Tekanan Darah Pada Penderita Hipertensi Pengaruh Pemberian Air Perasan Buah Mengkudu (Morinda Citrifolia) Terhadap Penurunan Tekanan Darah Pada Penderita Hipertensi A. *Prosiding Seminar Nasional Biology for Life* 7(2): 117–123.
- Sari, I., Junaidin, & Pratiwi. 2020. *Studi Molecular Docking Senyawa Flavonoid Herba Kumis Kucing (Orthosiphon stamineus B.) Pada Reseptor Alpha Glukosidase Sebagai Antidiabetes Tipe 2*. 7(2): 54–60.
- Sato, W., Hitaoka, S., Inoue, K., Imai, M., Saio, T., Uchida, T., Shinzawa-Itoh, K., Yoshikawa, S., Yoshizawa, K., & Ishimori, K. 2016. Energetic mechanism of cytochrome c-cytochrome c oxidase electron transfer complex formation under turnover conditions revealed by mutational effects and docking simulation. *Journal of Biological Chemistry* 291(29): 15320–15331. <https://doi.org/10.1074/jbc.M115.708065>
- Saudale, F. Z., Lerrick, R. I., Parikesit, A. A., & Mariti, F. 2019. Chemistry teachers' awareness, understanding, and confidence toward computational tools for molecular visualization. *Jurnal Pendidikan IPA Indonesia* 8(4): 436–446. <https://doi.org/10.15294/jpii.v8i4.21437>
- Schleinkofer, K., Wang, T., & Wade, R. C. 2006. Molecular Docking. *Encyclopedic Reference of Genomics and Proteomics in Molecular Medicine* 443: 1149–1153. https://doi.org/10.1007/3-540-29623-9_3820
- Schopf, F. H., Biebl, M. M., & Buchner, J. 2017. The HSP90 chaperone machinery. *Nature Reviews Molecular Cell Biology* 18(6): 345–360. <https://doi.org/10.1038/nrm.2017.20>

- Serafini, M. R., Santos, R. C., Guimarães, A. G., Dos Santos, J. P. A., Da Conceição Santos, A. D., Alves, I. A., Gelain, D. P., De Lima Nogueira, P. C., Quintans-Júnior, L. J., Bonjardim, L. R., & De Souza Araújo, A. A. 2011. Morinda citrifolia linn leaf extract possesses antioxidant activities and reduces nociceptive behavior and leukocyte migration. *Journal of Medicinal Food* 14(10): 1159–1166. <https://doi.org/10.1089/jmf.2010.0254>
- Sevrioukova, I. F., & Poulosa, T. L. 2013. Understanding The Mechanism Of Cytochrome P450 3a4: Recent Advances And Remaining Problems. 42(9): <https://doi.org/10.1039/c2dt31833d>
- Shah, D., & Osipo, C. 2016. Cancer stem cells and HER2 positive breast cancer: The story so far. *Genes and Diseases* 3(2): 114–123. <https://doi.org/10.1016/j.gendis.2016.02.002>
- Sharma, K., Pachauri, S. D., Khandelwal, K., Ahmad, H., Arya, A., Biala, P., Agrawal, S., Pandey, R. R., Srivastava, A., Srivastav, A., Saxena, J. K., & Dwivedi, A. K. 2015. Anticancer Effects of Extracts from the Fruit of Morinda Citrifolia (Noni) in Breast Cancer Cell Lines. *Drug Research* 66(3): 141–147. <https://doi.org/10.1055/s-0035-1555804>
- Sharma, V., & Sarkar, I. N. 2012. Bioinformatics opportunities for identification and study of medicinal plants. *Briefings in Bioinformatics* 14(2): 238–250. <https://doi.org/10.1093/bib/bbs021>
- Shi, J., Van De Water, R., Hong, K., Lamer, R. B., Weichert, K. W., Sandoval, C. M., Kasibhatla, S. R., Boehm, M. F., Chao, J., Lundgren, K., Timple, N., Lough, R., Ibanez, G., Boykin, C., Burrows, F. J., Kehry, M. R., Yun, T. J., Harning, E. K., Ambrose, C., ... Biamonte, M. A. 2012. EC144 is a potent inhibitor of the heat shock protein 90. *Journal of Medicinal Chemistry* 55(17): 7786–7795. <https://doi.org/10.1021/jm300810x>
- Shi, L., Tong, W., & Lu, X.-P. 2003. Biochemoinformatics: Integrating Bioinformatics and Chemoinformatics for Drug Discovery and Development. *Current*.
- Shin, E. J., Choi, H. K., Sung, M. J., Park, J. H., Chung, M. Y., Chung, S., & Hwang, J. T. 2018. Anti-tumour effects of beta-sitosterol are mediated by AMPK/PTEN/HSP90 axis in AGS human gastric adenocarcinoma cells and xenograft mouse models. *Biochemical Pharmacology* 152: 60–70. <https://doi.org/10.1016/j.bcp.2018.03.010>
- Shin, H. K., Kang, M. G., Park, D., Park, T., & Yoon, S. 2020. Development of Prediction Models for Drug-Induced Cholestasis, Cirrhosis, Hepatitis, and

- Steatosis Based on Drug and Drug Metabolite Structures. *Frontiers in Pharmacology* 11. <https://doi.org/10.3389/fphar.2020.00067>
- Sienkiewicz-Oleszkiewicz, B., & Wiela-Hojeńska, A. 2018. CYP2C19 polymorphism in relation to the pharmacotherapy optimization of commonly used drugs. *Pharmazie* 73(11): 619–624. <https://doi.org/10.1691/ph.2018.8689>
- Sogandi, S., Fitrianingrum, M., & Thursina, A. 2020. Identifikasi Senyawa Bioaktif dan Aktivitas Antibakteri Ekstrak Daun Mengkudu (*Morinda citrifolia* L.) sebagai Inhibitor *Propionibacterium acne*. *Buletin Penelitian Kesehatan* 48(1): 73–82. <https://doi.org/10.22435/bpk.v48i1.2338>
- Su, B. N., Pawlus, A. D., Jung, H. A., Keller, W. J., McLaughlin, J. L., & Kinghorn, A. D. 2005. Chemical constituents of the fruits of *Morinda citrifolia* (Noni) and their antioxidant activity. *Journal of Natural Products* 68(4): 592–595. <https://doi.org/10.1021/np0495985>
- Sun, H. 2004. A universal molecular descriptor system for prediction of LogP, LogS, LogBB, and absorption. *Journal of Chemical Information and Computer Sciences* 44(2): 748–757. <https://doi.org/10.1021/ci030304f>
- Suryadi Budi Utomo, Fajar Sanubari, Budi Utami, dan N. D. N., & Program. 2017. Aktivitas Analgesik Senyawa Turunan Meperidin Menggunakan Metode Semiempiris AM1 Analysis of a Quantitative Relationship Between the Structure and Analgesic Activity of Meperidin Derivatives Using. (*Jurnal Kimia Dan Pendidikan Kimia*, 2(3): 158–168.
- Suvannang, N., Nantasenamat, C., Isarankura-Na-Ayudhya, C., & Prachayasittikul, V. 2011. Molecular docking of *aromatase* inhibitors. *Molecules* 16(5): 3597–3617. <https://doi.org/10.3390/molecules16053597>
- Swamy, K. V., & Padhye, S. 2011. *Molecular Docking Studies On Estrogen Receptor - α And Chalcone Derivatives Available Online through* 1(3): 87–93.
- Syahputra, G., Ambarsari L, & T, S. 2014. Simulasi docking kurkumin enol, bisdemetoksikurkumin dan analognya sebagai inhibitor enzim 12-lipoksigenase. *Biofisika* 10(1): 55–67.
- Tanriono, S., Rotty, L. W. A., & Haroen, H. 2012. Breast Cancer Histopathology For January 2012 - December 2012 2(1): 1-6

- Tecalco-Cruz, A. C., & Ramírez-Jarquín, J. O. 2017. Mechanisms that Increase Stability of Estrogen Receptor Alpha in Breast Cancer. *Clinical Breast Cancer* 17(1): 1–10. <https://doi.org/10.1016/j.clbc.2016.07.015>
- Tegar, M., & Purnomo, H. 2013. Tea Leaves Extracted as Anti-Malaria based on Molecular Docking PLANTS. *Procedia Environmental Sciences* 17: 188–194. <https://doi.org/10.1016/j.proenv.2013.02.028>
- Thakuria, R., Nath, N. K., & Saha, B. K. 2019. The Nature and Applications of π - π Interactions: A Perspective. *Crystal Growth and Design* 19(2): 523–528. <https://doi.org/10.1021/acs.cgd.8b01630>
- Thani, W., Vallisuta, O., Siripong, P., & Ruangwises, N. 2010. Anti-proliferative and antioxidative activities of Thai noni/Yor (*Morinda citrifolia* Linn.) leaf extract. *Southeast Asian Journal of Tropical Medicine and Public Health* 41(2): 482–489.
- Thani, W., Vallisuta, O., Siripong, P., & Ruangwises, N. 2010. Anti-proliferative and antioxidative activities of Thai noni/Yor (*Morinda citrifolia* Linn.) leaf extract. *Southeast Asian Journal of Tropical Medicine and Public Health* 41(2): 482–489.
- Toutain, P. L., & Bousquet-Mélou, A. 2004. Volumes of distribution. *Journal of Veterinary Pharmacology and Therapeutics* 27(6): 441–453. <https://doi.org/10.1111/j.1365-2885.2004.00602.x>
- Van Breemen, R. B., & Li, Y. 2005. Caco-2 cell permeability assays to measure drug absorption. *Expert Opinion on Drug Metabolism and Toxicology* 1(2): 175–185. <https://doi.org/10.1517/17425255.1.2.175>
- Wanat, K. 2020. Biological barriers, and the influence of protein binding on the passage of drugs across them. *Molecular Biology Reports* 47(4): 3221–3231. <https://doi.org/10.1007/s11033-020-05361-2>
- Wang, A., Stout, C. D., Zhang, Q., & Johnson, E. F. 2015. Contributions of ionic interactions and protein dynamics to cytochrome P450 2D6 (CYP2D6) substrate and inhibitor binding. *Journal of Biological Chemistry* 290(8): 5092–5104. <https://doi.org/10.1074/jbc.M114.627661>
- Wang, G. X., Zhang, H., He, F. F., & Fang, X. M. 2006. Effect of the CYP2D6*10 C188T polymorphism on postoperative tramadol analgesia in a Chinese population. *European Journal of Clinical Pharmacology* 62(11): 927–931. <https://doi.org/10.1007/s00228-006-0191-2>

- Wang, J., & Hou, T. 2011. Recent Advances on Aqueous Solubility Prediction. *Combinatorial Chemistry & High Throughput Screening* 14(5): 328–338. <https://doi.org/10.2174/138620711795508331>
- Wang, L., Ding, L., Du, Z., & Liu, J. 2020. Effects of hydrophobicity and molecular weight on the transport permeability of oligopeptides across Caco-2 cell monolayers. *Journal of Food Biochemistry* 44(5): 1–8. <https://doi.org/10.1111/jfbc.13188>
- Wang, Y., Xiao, Q., Chen, P., & Wang, B. 2019. In silico prediction of drug-induced liver injury based on ensemble classifier method. *International Journal of Molecular Sciences* 20(17): 1–13. <https://doi.org/10.3390/ijms20174106>
- Wang, Z., Liang, L., Yin, Z., & Lin, J. 2016. Improving chemical similarity ensemble approach in target prediction. *Journal of Cheminformatics* 8(1): 1–10. <https://doi.org/10.1186/s13321-016-0130-x>
- Watroly, M. N., Sekar, M., Fuloria, S., Gan, S. H., Jeyabalan, S., Wu, Y. S., Subramaniyan, V., Sathasivam, K. V. 2021. Chemistry, biosynthesis, physicochemical and biological properties of rubiadin: A promising natural anthraquinone for new drug discovery and development. *Drug Design, Development and Therapy*, 15: 4527–4549. <https://doi.org/10.2147/DDDT.S338548>
- Wen, M., Deng, Z. K., Jiang, S. L., Guan, Y. Di, Wu, H. Z., Wang, X. L., Xiao, S. S., Zhang, Y., Yang, J. M., Cao, D. S., & Cheng, Y. 2019. Identification of a Novel Bcl-2 Inhibitor by Ligand-Based Screening and Investigation of Its Anti-cancer Effect on Human Breast Cancer Cells. *Frontiers in Pharmacology* 10: 1–14. <https://doi.org/10.3389/fphar.2019.00391>
- Wen, M., Deng, Z. K., Jiang, S. L., Guan, Y. Di, Wu, H. Z., Wang, X. L., Xiao, S. S., Zhang, Y., Yang, J. M., Cao, D. S., & Cheng, Y. 2019. Identification of a Novel Bcl-2 Inhibitor by Ligand-Based Screening and Investigation of Its Anti-cancer Effect on Human Breast Cancer Cells. *Frontiers in Pharmacology* 10: 1–14. <https://doi.org/10.3389/fphar.2019.00391>
- Werk, A. N., & Cascorbi, I. 2014. Functional gene variants of CYP3A4. *Clinical Pharmacology and Therapeutics* 96(3): 340–348. <https://doi.org/10.1038/clpt.2014.129>
- WHO. 2021. Breast cancer now most common form of cancer: WHO taking action. Departmental News. <https://www.who.int/news/item/03-02-2021-breast-cancer-now-most-common-form-of-cancer-who-taking-action>. 10 Maret 2021 (14:30).

- Wigati, D., Anwar, K., Sudarsono, & Nugroho, A. E. 2017. Hypotensive Activity of Ethanolic Extracts of *Morinda citrifolia* L. Leaves and Fruit in Dexamethasone-Induced Hypertensive Rat. *Journal of Evidence-Based Complementary and Alternative Medicine* 22(1): 107–113. <https://doi.org/10.1177/2156587216653660>
- Xiong, G., Wu, Z., Yi, J., Fu, L., Yang, Z., Hsieh, C., Yin, M., Zeng, X., Wu, C., Lu, A., Chen, X., Hou, T., & Cao, D. 2021. ADMETlab 2.0: An integrated online platform for accurate and comprehensive predictions of ADMET properties. *Nucleic Acids Research* 49(1): 5–14. <https://doi.org/10.1093/nar/gkab255>
- Yan, A., Wang, Z., & Cai, Z. 2008. Prediction of human intestinal absorption by GA feature selection and support vector machine regression. *International Journal of Molecular Sciences* 9(10): 1961–1976. <https://doi.org/10.3390/ijms9101961>
- Yan, L., Rosen, N., & Arteaga, C. 2011. Targeted cancer therapies. *Chinese Journal of Cancer* 30(1): 1–4. <https://doi.org/10.5732/cjc.010.10553>
- Youn, U. J., & Chang, L. C. 2017. Chemical constituents of fermented noni (*Morinda citrifolia*) juice exudates and their biological activity. *Natural Product Sciences* 23(1): 16–20. <https://doi.org/10.20307/nps.2017.23.1.16>
- Yue, W., Yager, J. D., Wang, J. P., Jupe, E. R., & Santen, R. J. 2013. Estrogen receptor-dependent and independent mechanisms of breast cancer carcinogenesis. *Steroids* 78(2): 161–170. <https://doi.org/10.1016/j.steroids.2012.11.001>
- Zagouri, F., Bournakis, E., Koutsoukos, K., & Papadimitriou, C. A. 2012. Heat shock protein 90 (HSP90) expression and breast cancer. *Pharmaceuticals* 5(9): 1008–1020. <https://doi.org/10.3390/ph5091008>
- Zanger, U. M., & Schwab, M. 2013. Cytochrome P450 enzymes in drug metabolism: Regulation of gene expression, enzyme activities, and impact of genetic variation. *Pharmacology and Therapeutics* 138(1): 103–141. <https://doi.org/10.1016/j.pharmthera.2012.12.007>
- Zhao, C., She, T., Wang, L., Su, Y., Qu, L., Gao, Y., Xu, S., Cai, S., & Shou, C. 2015. Daucosterol inhibits cancer cell proliferation by inducing autophagy through reactive oxygen species-dependent manner. *Life Sciences* 137: 37–43. <https://doi.org/10.1016/j.lfs.2015.07.019>
- Zhivkova, Z., & Doytchinov, I. 2012. Quantitative Structure—Plasma Protein Binding Relationships of Acidic Drugs. *Journal of Pharmaceutical Sciences*, 101(7): 2271–2280. <https://doi.org/10.1002/jps>

Zhou, K., Donnelly, L., Burch, L., Tavendale, R., Doney., Morris, A. D., & Pearson, E. R. 2010. Loss-of-function CYP2C9 variants improve therapeutic response to sulfonylureas in type 2 diabetes: A go-DARTS study. *Clinical Pharmacology and Therapeutics* 87(1): 52–56. <https://doi.org/10.1038/clpt.2009.176>