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Gc-ms-and nmr-based metabolomics and molecular docking reveal the potential alpha-glucosidase inhibitors from psychotria malayana jack leaves

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Abstract

Psychotria malayana Jack leaf, known in Indonesia as “daun salung”, is traditionally used for the treatment of diabetes and other diseases. Despite its potential, the phytochemical study related to its anti-diabetic activity is still lacking. Thus, this study aimed to identify putative inhibitors of α-glucosidase, a prominent enzyme contributing to diabetes type 2 in P. malayana leaf extract using gas chromatography-mass spectrometry (GC-MS)-and nuclear magnetic resonance (NMR)-based metabolomics, and to investigate the molecular interaction between those inhibitors and the enzyme through in silico approach. Twenty samples were extracted with different solvent ratios of methanol– water (0, 25, 50, 75, and 100% v/v). All extracts were tested on the alpha-glucosidase inhibition (AGI) assay and analyzed using GC-MS and NMR. Multivariate data analysis through a partial least square (PLS) and orthogonal partial square (OPLS) models were developed in order to correlate the metabolite profile and the bioactivity leading to the annotation of the putative bioactive compounds in the plant extracts. A total of ten putative bioactive compounds were identified and some of them reported in this plant for the first time, namely 1,3,5-benzenetriol (1); palmitic acid (2); cholesta-7,9(11)-diene-3-ol (3); 1-monopalmitin (4); β-tocopherol (5); α-tocopherol (6); 24-epicampesterol (7); stigmast-5-ene (8); 4-hydroxyphenylpyruvic acid (10); and glutamine (11). For the evaluation of the potential binding modes between the inhibitors and protein, the in silico study via molecular docking was performed where the crystal structure of Saccharomyces cerevisiae isomaltase (PDB code: 3A4A) was used. Ten amino acid residues, namely ASP352, HIE351, GLN182, ARG442, ASH215, SER311, ARG213, GLH277, GLN279, and PRO312 established hydrogen bond in the docked complex, as well as hydrophobic interaction of other amino acid residues with the putative compounds. The α-glucosidase inhibitors showed moderate to high binding affinities (−5.5 to −9.4 kcal/mol) towards the active site of the enzymatic protein, where compounds 3, 5, and 8 showed higher binding affinity compared to both quercetin and control ligand.

Author Keywords

GC-MS; Molecular docking; Multivariate data analysis; NMR; P. malayana; α-glucosidase

References

- Murugesu, S., Ibrahim, Z., Ahmed, Q.-U., Yusoff, N.-I.N., Uzir, B.-F., Perumal, V., Abas, F., Khatib, A.
  Characterization of α-glucosidase inhibitors from Clinacanthus nutans lindau leaves by gas chromatography-mass spectrometry-based metabolomics and molecular docking simulation

(2018) *Molecules*, 23, p. 2402.
[CrossRef]

- Saeedi, P., Petersohn, I., Salpea, P., Malanda, B., Karuranga, S., Unwin, N., Colagiuri, S., Ogurtsova, K.
Global and regional diabetes prevalence estimates for 2019 and projections for 2030 and 2045: Results from the International Diabetes Federation Diabetes Atlas, 9th Edition
(2019) *Diabetes Res. Clin. Pract*, 157, p. 107843.
[CrossRef] [PubMed]

- Nair, S.S., Kavrekar, V., Mishra, A.
In vitro studies on alpha amylase and alpha glucosidase inhibitory activities of selected plant extracts
(2013) *Eur. J. Exp. Biol*, 3, pp. 128-132.

- Graham, J.E., Stoebner-may, D.G., Ostir, G.V., Al, S., Peek, M.K., Markides, K., Ottenbacher, K.J.
Health related quality of life in older Mexican Americans with diabetes: A cross-sectional study
(2007) *Health Qual. Life Outcomes*, 5, p. 39.
[CrossRef] [PubMed]

- Haque, N., Salma, U., Nurunnabi, T.R., Uddin, M.J., Jahangir, M.F.K., Islam, S.M.Z., Kamruzzaman, M.
Management of Type 2 Diabetes mellitus by lifestyle, diet and medicinal plants
(2011) *Pakistan J. Biol. Sci*, 14, pp. 13-24.
[CrossRef] [PubMed]

- Gro, J.K., Yada, S., Vats, V.
Medicinal Plants of India with Anti-Diabetic Potential
(2002) *J. Ethnopharmacol*, 81, pp. 81-100.

- Situmorang, R.O.P., Harianja, A.H., Silalahi, J.
Karo's Local Wisdom: The use of woody plants for traditional diabetic medicines
(2015) *Indones. J. For. Res*, 2, pp. 121-130.
[CrossRef]

- Hadi, S., Asnawati, D., Ersalena, V.F., Azwari, A., Rahmawati, K.P.
Characterization of alkaloids from the leaves of Psychotria malayana jack of Lombok island on the basis of gas chromatography-mass spectroscopy
(2014) *J. Pure Appl. Chem. Res*, 3, pp. 108-113.
[CrossRef]

- Matsuura, H.N., Porto, D.D., Fett-Neto, A.G.
Bioactive alkaloids from south american Psychotria and related rubiaceae
(2013) *Natural Products*, pp. 119-147.
Springer: Berlin/Heidelberg, Germany, [CrossRef]

- Chebib, M., Duke, R.K., Duke, C.C., Connor, M., Mewett, K.N., Johnston, G.A.R.
Convulsant actions of calycanthine
(2003) *Toxicol. Appl. Pharmacol*, 190, pp. 58-64.
[CrossRef]

- Hadi, S.
  (2002) *Bioactive Alkaloids from Medicinal Plants of Lombok*,
  University of Wollongong: Wollongong, Australia

- Nokhala, A., Siddiqui, M.J., Ahmed, Q.U., Bustamam, M.S.A., Zakaria, Z.A.
  Investigation of α-glucosidase inhibitory metabolites from Tetracera scandens leaves by GC–MS metabolite profiling and docking studies
  (2020) *Biomolecules*, 10, p. 287.
  [CrossRef]

- Eriksson, L., Byrne, T., Johansson, E., Trygg, J., Vikström, C.
  (2006) *Multi-and Megavariate Data Analysis Basic Principles and Applications*,
  2nd ed.; Umetrics Academy: Umea, Sweden

- Javadi, N., Abas, F., Hamid, A.A., Simoh, S., Shaari, K., Ismail, I.S., Mediani, A., Khatib, A.
  GC-MS-based metabolite profiling of Cosmos caudatus leaves possessing alpha-glucosidase inhibitory activity
  (2014) *J. Food Sci*, 79, pp. C1130-C1136.
  [CrossRef]

- Das, S., Dutta, M., Chaudhury, K., De, B.
  Metabolomic and Chemometric Study of Achras Sapota L. Fruit extracts for identification of metabolites contributing to the inhibition of α-amylase and α-glucosidase
  (2016) *Eur. Food Res. Technol*, 242, pp. 733-743.
  [CrossRef]

- Tan, D.C., Kassim, N.K., Ismail, I.S., Hamid, M., Ahamad Bustamam, M.S.
  Identification of antidiabetic metabolites from Paederia foetida l. twigs by gas chromatography-mass spectrometry-based metabolomics and molecular docking study
  (2019) *Biomed. Res. Int*, 2019, p. 7603125.
  [CrossRef]

- Markley, J.L., Brüschweiler, R., Edison, A.S., Eghbalnia, H.R., Powers, R., Raftery, D., Wishart, D.S.
  The future of NMR-based metabolomics
  (2017) *Curr. Opin. Biotechnol*, 43, pp. 34-40.
  [CrossRef]

- Zolkeflee, N.K.Z., Isamail, N.A., Maulidiani, M., Abdul Hamid, N.A., Ramli, N.S., Azlan, A., Abas, F.
  Metabolite variations and antioxidant activity of Muntingia calabura leaves in response to different drying methods and ethanol ratios elucidated by NMR-based metabolomics
  (2020) *Phytochem. Anal*, 32, pp. 69-83.
  [CrossRef] [PubMed]

- Sussulini, A.
  (2017) *Metabolomics: From Fundamentals to Clinical Applications*,
  (Ed) 1st ed.; Springer: Gewerbestrasse, Switzerland, [CrossRef]

- Mediani, A., Abas, F., Maulidiani, M., Khatib, A., Tan, C.P., Safinar Ismail, I., Shaari, K., Ismail, A.
  Characterization of metabolite profile in Phyllanthus niruri and correlation with bioactivity elucidated by nuclear magnetic resonance based metabolomics
  (2017) *Molecules*, 22, p. 902.
  [CrossRef] [PubMed]

- Atanasov, A.G., Waltenberger, B., Pferschy-Wenzig, E.M., Linder, T., Wawrosch, C., Uhrin, P., Temml, V., Heiss, E.H.
  Discovery and resupply of pharmacologically active plant-derived natural products: A review
  (2015) *Biotechnol. Adv*, 33, pp. 1582-1614.
  [CrossRef] [PubMed]

- Singla, R.K., Dubey, A.K.
  Phytochemical Profiling, GC-MS analysis and α-amylase inhibitory potential of ethanolic extract of Cocos Nucifera Linn
  (2019) *Endocarp. Endocr. Metab. Immune Disord.-Drug Targets*, 19, pp. 419-442.
  [CrossRef]

- Jardim, C.M., Jham, G.N., Dhingra, O.D., Freire, M.M.
  Composition and antifungal activity of the essential oil of the brazilian Chenopodium Ambrosioides L
  (2008) *J. Chem. Ecol*, 34, pp. 1213-1218.
  [CrossRef] [PubMed]

- Efron, B., Gong, G.
  A Leisurely Look at the Bootstrap, the Jackknife, and Cross-Validation
  (1983) *Am. Stat*, 37, pp. 36-48.

- Kim, H.K., Choi, Y.H., Verpoorte, R.
  NMR-based metabolomics analysis of plants
  (2010) *Nat. Protoc*, 5, pp. 536-549.
  [CrossRef] [PubMed]

- Choi, Y.H., Kim, H.K., Linthorst, H.J.M., Hollander, J.G., Lefeber, A.W.M., Erkelens, C., Nuzillard, J.M., Verpoorte, R.
  NMR metabolomics to revisit the Tobacco Mosaic virus infection in Nicotiana tabacum leaves
  (2006) *J. Nat. Prod*, 69, pp. 742-748.
  [CrossRef] [PubMed]

- Lee, I.J., Hom, K., Bai, G., Shapiro, M.
  NMR metabolomics analysis of caco-2 cell differentiation
  (2009) *J. Proteome Res*, 8, pp. 4104-4108.
  [CrossRef] [PubMed]

- Jindra, A., Šípal, Z., Hudecová, V.
  Biosynthesis of Alkaloids. On the occurrence of keto acids in Papaver Somniferum L. plants
  (1964) *Experientia*, 20, pp. 371-372.
  [CrossRef]

- Hou, Z., Li, Y., Su, F., Chen, J., Zhang, X., Xu, L., Yang, D., Liang, Z.
Application of 1H-NMR Combined with QRT-PCR technology in the exploration of rosmarinic acid biosynthesis in hair roots of Salvia miltiorrhiza Bunge and Salvia castanea f. Tomentosa Stib
(2021) *Planta*, 253, p. 2.
[CrossRef]

- Kuo, Y.H., Ikegami, F., Lambein, F.
Neuroactive and other free amino acids in seed and young plants of Panax ginseng
(2003) *Phytochemistry*, 62, pp. 1087-1091.
[CrossRef]

- Peksa, A., Miedzianka, J., Nems, A., Rytel, E.
The free-amino-acid content in six potatoes cultivars through storage
(2021) *Molecules*, 26, p. 1322.
[CrossRef]

- Khoo, L.W., Mediani, A., Zolkeflee, N.K.Z., Leong, S.W., Ismail, I.S., Khatib, A., Shaari, K., Abas, F.
Phytochemical diversity of Clinacanthus nutans extracts and their bioactivity correlations elucidated by NMR based metabolomics
(2015) *Phytochem. Lett*, 14, pp. 123-133.
[CrossRef]

- Maroyi, A.
Hilliardiella Elaeagnoides: Review of its medicinal uses, phytochemistry and pharmacological properties
(2020) *Res. J. Pharm. Technol*, 13, pp. 5539-5545.
[CrossRef]

- Nowakowski, P., Naliwajko, S.K., Markiewicz-Żukowska, R., Borawska, M.H., Socha, K.
The two faces of Coprinus Comatus— functional properties and potential hazards
(2020) *Phyther. Res*, 34, pp. 2932-2944.
[CrossRef]

- Maulidiani, H., Khatib, A., Shaari, K., Abas, F., Shitan, M., Kneer, R., Neto, V., Lajis, N.H.
Discrimination of three pegaga (centella) varieties and determination of growth-lighting effects on metabolites content based on the chemometry of 1h nuclear magnetic resonance spectroscopy
(2012) *J. Agric. Food Chem*, 60, pp. 410-417.
[CrossRef]

- Mediani, A., Abas, F., Khatib, A., Tan, C.P., Ismail, I.S., Shaari, K., Ismail, A., Lajis, N.H.
Phytochemical and biological features of Phyllanthus niruri and Phyllanthus urinaria harvested at different growth stages revealed by 1h NMR-based metabolomics
(2015) *Ind. Crops Prod*, 77, pp. 602-613.
[CrossRef]

- Wei, S., Abas, F., Wai, K., Yusoff, K.
In Vitro and In Silico Evaluations of diarylpentanoid series as α-glucosidase inhibitor
(2018) *Bioorg. Med. Chem. Lett*, 28, pp. 302-309.
[CrossRef]

- Kidane, Y., Bokrezion, T., Mebrahtu, J., Mehari, M., Gebreab, Y.B., Fessehaye, N., Achila, O.O.
  In vitro inhibition of α-amylase and α-glucosidase by extracts from Psiadia punctulata and Meriandra bengalensis
  (2018) *Evid.-Based Complement Altern. Med*, 2018, pp. 1-9.
  [CrossRef] [PubMed]

- Bhatia, A., Singh, B., Arora, R., Arora, S.
  In Vitro Evaluation of the α-glucosidase inhibitory potential of methanolic extracts of traditionally used antidiabetic plants
  (2019) *BMC Complement Altern. Med*, 19, p. 74.
  [CrossRef] [PubMed]

- Sharif, M.F., Bennett, M.T.
  The Effect of different methods and solvents on the extraction of polyphenols in ginger (Zingiber officinale)
  (2016) *J. Teknol*, 78, pp. 49-54.
  [CrossRef]

- Nipun, T.S., Khatib, A., Ahmed, Q.U., Redzwan, I.E., Ibrahim, Z., Khan, A.Y.F., Primaharinastiti, R., El-Seedi, H.R.
  Alpha-glucosidase inhibitory effect of Psychotria malayana jack leaf: A rapid analysis using infrared fingerprinting
  (2020) *Molecules*, 25, p. 4161.
  [CrossRef]

- Prihantini, A.I., Tachibana, S., Itoh, K.
  Evaluation of Antioxidant and α-Glucosidase Inhibitory Activities of Some Subtropical Plants
  (2014) *Pak. J. Biol. Sci*, 17, pp. 1106-1114.
  [CrossRef]

- Indrianingsih, A.W., Tachibana, S., Itoh, K.
  In Vitro Evaluation of Antioxidant and α-Glucosidase Inhibitory Assay of Several Tropical and Subtropical Plants
  (2015) *Procedia Environ. Sci*, 28, pp. 639-648.
  [CrossRef]

- Dirir, A.M., Daou, M., Yousef, A.F., Yousef, L.F.
  A Review of Alpha-Glucosidase Inhibitors from Plants as Potential Candidates for the Treatment of Type-2 Diabetes
  (2021) *Phytochem. Rev*,
  [CrossRef]

- Mauldina, M.G., Sauriasari, R., Elya, B.
  α-Glucosidase Inhibitory Activity from Ethyl Acetate Extract of Antidesma Bunius (L.) Spreng Stem Bark Containing Triterpenoids
  (2017) *Pharmacogn. Mag*, 13, pp. 590-594.
  [CrossRef]

- Ankita Bachhawat, J., Shihabudeen, M.S., Thirumurugan, K.
  Screening of Fifteen Indian Ayurvedic Plants for Alpha-Glucosidase Inhibitory Activity and Enzyme Kinetics
  (2011) *Int. J. Pharm. Pharm. Sci*, 3, pp. 267-274.

- Alam, M.A., Zaidul, I.S.M., Ghafoor, K., Sahena, F., Hakim, M.A., Rafii, M.Y., Abir, H.M., Khatib, A.
  In vitro antioxidant and, α-glucosidase inhibitory activities and comprehensive metabolite profiling of methanol extract and its fractions from Clinacanthus nutans
  (2017) *BMC Complement Altern. Med*, 17, p. 181.
  [CrossRef] [PubMed]

- Javadi, N., Abas, F., Mediani, A., Abd Hamid, A., Khatib, A., Simoh, S., Shaari, K.
  Effect of Storage Time on metabolite profile and alpha-glucosidase inhibitory activity of Cosmos caudatus leaves-GCMS based metabolomics approach
  (2015) *J. Food Drug Anal*, 23, pp. 433-441.
  [CrossRef] [PubMed]

- Yumna, M., Angelina, Abdullah, Arbianti, R., Utami, T.S., Hermansyah, H.
  Effect of mother-in-law's tongue leaves (Sansevieria trifasciata) extract's solvent polarity on anti-diabetic activity through in vitro α-glucosidase enzyme inhibition test
  (2018) *E3S Web of Conferences*, 67, pp. 1-5.
  Auffret-Babak, I., Ed.; EDP Sciences: Paris, Franch, [CrossRef]

- Srilatha, B.R., Ananda, S.
  Antidiabetic Effects of Mukia Maderaspatana and Its Phenolics: An in vitro study on gluconeogenesis and glucose uptake in rat tissues
  (2014) *Pharm. Biol*, 52, pp. 597-602.
  [CrossRef] [PubMed]

- Yoon, J.Y., Choi, H., Jun, H.S.
  The Effect of phloroglucinol, a component of Ecklonia cava extract, on hepatic glucose production
  (2017) *Mar. Drugs*, 15, p. 106.
  [CrossRef] [PubMed]

- Akhtar, M., Freeman, C.W., Rahimtula, A.D., Wilton, D.C.
  A Novel olefinic rearrangement the enzymic conversion of cholesta-7,9-dien-3β-ol into cholesta-8,14-dien-3β-ol
  (1972) *Biochem. J*, 129, pp. 225-229.
  [CrossRef]

- Jamaluddin, F., Mohamed, S., Lajis, M.N.
  Hypoglycaemic effect of Parkia speciosa seeds due to the synergistic action of β-sitosterol and stigmasterol
  (1994) *Food Chem*, 49, pp. 339-345.
  [CrossRef]

- Kuhlisch, C., Pohnert, G.
  Metabolomics in chemical ecology
  (2015) *Nat. Prod. Rep*, 32, pp. 937-955.
  [CrossRef]

- Salem, M.A., De Souza, L.P., Serag, A., Fernie, A.R., Farag, M.A., Ezzat, S.M., Alseekh, S.
  Metabolomics in the context of plant natural products research: From sample preparation to metabolite analysis

(2020) *Metabolites*, 10, p. 37.
[CrossRef]

- Shi, M., Huang, F., Deng, C., Wang, Y., Kai, G.
Bioactivities, biosynthesis and biotechnological production of phenolic acids in Salvia miltiorrhiza
(2018) *Crit. Rev. Food Sci. Nutr*, 59, pp. 953-964.
[CrossRef]

- Białecka-Florjańczyk, E., Fabiszewska, A., Zieniuk, B.
Phenolic acids derivatives-biotechnological methods of synthesis and bioactivity
(2018) *Curr. Pharm. Biotechnol*, 19, pp. 1098-1113.
[CrossRef] [PubMed]

- Wang, C., Deng, Y., Yue, Y., Chen, W., Zhang, Y., Shi, G., Wu, Z.
Glutamine enhances the hypoglycemic effect of insulin in l6 cells via phosphatidylinositol-3-kinase (PI3K)/protein kinase B (AKT)/glucose transporter 4 (GLUT4) signaling pathway
(2018) *Med. Sci. Monit*, 24, pp. 1241-1250.
[CrossRef]

- Jafari-Vayghan, H., Varshosaz, P., Hajizadeh-Sharafabad, F., Razmi, H.R., Amirpour, M., Tavakoli-Rouzbehani, O.M., Alizadeh, M., Maleki, V.
A Comprehensive insight into the effect of glutamine supplementation on metabolic variables in diabetes mellitus: A systematic review
(2020) *Nutr. Metab*, 17, p. 80.
[CrossRef] [PubMed]

- Samocha-Bonet, D., Chisholm, D.J., Gribble, F.M., Coster, A.C.F., Carpenter, K.H., Jones, G.R.D., Holst, J.J., Greenfield, J.R.
Glycemic effects and safety of l-glutamine supplementation with or without sitagliptin in type 2 diabetes patients-a randomized study
(2014) *PLoS ONE*, 9, p. e113366.
[CrossRef]

- Yang, G., Zhang, Y., Wu, D., Wang, C., Yang, Y.J., Fan, S.J., Xia, L., Peng, X.
1H-NMR metabolomics identifies significant changes in hypermetabolism after glutamine administration in burned rats
(2019) *Am. J. Transl. Res*, 11, pp. 7286-7299.
[PubMed]

- Wei, S., Liu, L., Zhang, J., Bowers, J., Gowda, G.A.N., Seeger, H., Fehm, T., Clare, S.E.
Metabolomics approach for predicting response to neoadjuvant chemotherapy for breast cancer
(2013) *Mol. Oncol*, 7, pp. 297-307.
[CrossRef] [PubMed]

- Cappello, T., Giannetto, A., Parrino, V., De Marco, G., Mauceri, A., Maisano, M.
Food safety using NMR-based metabolomics: Assessment of the Atlantic bluefin tuna, Thunnus thynnus, from the Mediterranean sea
(2018) *Food Chem. Toxicol*, 115, pp. 391-397.
[CrossRef]

- Yamamoto, K., Miyake, H., Kusunoki, M., Osaki, S.
  Crystal structures of isomaltase from Saccharomyces cerevisiae and in complex with its competitive inhibitor maltose
  (2010) *FEBS J*, 277, pp. 4205-4214.
  [CrossRef]

- Murugesu, S., Ibrahim, Z., Uddin, Q., Uzir, B.F., Nik, N.I., Perumal, V., Abas, F., Khatib, A.
  Identification of α-glucosidase inhibitors from Clinacanthus nutans leaf extract using liquid chromatography-mass spectrometry-based metabolomics and protein-ligand interaction with molecular docking
  (2019) *J. Pharm. Anal*, 9, pp. 91-99.
  [CrossRef]

- Ali, M.Y., Kim, D.H., Seong, S.H., Kim, H.-R., Jung, H.A., Choi, J.S.
  α-Glucosidase and protein tyrosine phosphatase 1b inhibitory activity of plastoquinones from marine brown alga Sargassum serratifolium
  (2017) *Mar. Drugs*, 15, p. 368.
  [CrossRef]

- Seong, S.H., Roy, A., Jung, H.A., Jung, H.J., Choi, J.S.
  Protein tyrosine phosphatase 1b and α-glucosidase inhibitory activities of Pueraria lobata root and its constituents
  (2016) *J. Ethnopharmacol*, 194, pp. 706-716.
  [CrossRef]

- Nipun, T.S., Khatib, A., Ibrahim, Z., Ahmed, Q.U., Redzwan, I.E., Saiman, M.Z., Supandi, F., El-Seedi, H.R.
  Characterization of α-glucosidase inhibitors from Psychotria malayana jack leaves extract using LC-MS-based multivariate data analysis and in-silico molecular docking
  (2020) *Molecules*, 25, p. 5885.
  [CrossRef]

- Chen, Y.C.
  Beware of docking!
  (2014) *Trends Pharmacol. Sci*, 36, pp. 78-95.
  [CrossRef]

- Vieira, T.F., Sousa, S.F.
  Comparing autodock and vina in ligand/decoy discrimination for virtual screening
  (2019) *Appl. Sci*, 9, p. 4538.
  [CrossRef]

- Gupta, A., Narkowicz, C.K., Al-Aubaidy, H.A., Jelinek, H.F., Nichols, D.S., Burgess, J.R., Jacobson, G.A.
  Phytosterol supplements do not inhibit dipeptidyl peptidase-4
  (2020) *Diabetes Metab. Syndr. Clin. Res. Rev*, 14, pp. 1475-1478.
  [CrossRef] [PubMed]

- Taha, M., Adnan, S., Shah, A., Afifi, M., Imran, S., Sultan, S., Rahim, F., Mohammed, K.
  Synthesis, α-glucosidase inhibition and molecular docking study of coumarin based derivatives
  (2018) *Bioorg. Chem*, 77, pp. 586-592.
  [CrossRef] [PubMed]

- Alyar, S., Sen, T., Ozmen, Ü.O., Alyar, H., Adem, S., Sen, C.
Synthesis, spectroscopic characterizations, enzyme inhibition, molecular docking study and dft calculations of new schiff bases of sulfa drugs
(2019) *J. Mol. Struct*, 1185, pp. 416-424.
[CrossRef]

- Patil, R., Das, S., Stanley, A., Yadav, L., Sudhakar, A., Varma, A.K.
Optimized hydrophobic interactions and hydrogen bonding at the target-ligand interface leads the pathways of drug-designing
(2010) *PLoS ONE*, 5, p. e12029.
[CrossRef]

- Han, L., Fang, C., Zhu, R., Peng, Q., Li, D., Wang, M.
Inhibitory effect of phloretin on α-glucosidase: Kinetics, interaction mechanism and molecular docking
(2017) *Int. J. Biol. Macromol*, 95, pp. 520-527.
[CrossRef]

- Imran, S., Taha, M., Ismail, H., Kashif, S.M., Rahim, F., Jamil, W., Wahab, H., Khan, K.M.
Synthesis, In vitro and docking studies of new flavone ethers as α-glucosidase inhibitors
(2016) *Chem. Biol. Drug Des*, 87, pp. 361-373.
[CrossRef] [PubMed]

- Lestari, W., Dewi, R.T., Broto, L., Kardono, S., Yanuar, A.
Docking sulochrin and its derivative as α-glucosidase inhibitors of Saccharomyces cerevisiae
(2017) *Indones. J. Chem*, 17, pp. 144-150.
[CrossRef]

- Yan, J., Zhang, G., Pan, J., Wang, Y.
α-Glucosidase inhibition by luteolin: Kinetics, interaction and molecular docking
(2014) *Int. J. Biol. Macromol*, 64, pp. 213-223.
[CrossRef] [PubMed]

- Leong, S.W., Awin, T., Munirah, S., Faudzi, M., Shaari, M.M.K., Abas, F.
Synthesis and biological evaluation of asymmetrical diarylpentanoids as antiin fl ammatory, anti-α-glucosidase, and antioxidant agents
(2019) *Med. Chem. Res*, 28, pp. 2002-2009.
[CrossRef]

- Dolinsky, T.J., Nielsen, J.E., Mccammon, J.A., Baker, N.A.
PDB2PQR: An automated pipeline for the setup of poisson–boltzmann electrostatics calculations
(2004) *Nucleic Acids Res*, 32, pp. 665-667.
[CrossRef] [PubMed]

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