Molecules • *Open Access* • Volume 28, Issue 15 • August 2023 • Article number 5752

Document type
Article • *Gold Open Access* • *Green Open Access*

Source type
Journal

ISSN
14203049

DOI
10.3390/molecules28155752

Publisher
Multidisciplinary Digital Publishing Institute (MDPI)

CODEN
MOLEF

Original language
English

PubMed ID
37570723

View less

Profiling the Antidiabetic Potential of Compounds Identified from Fractionated Extracts of Entada africana toward Glucokinase Stimulation: Computational Insight

Onikanni, Sunday Amos[a, b] ; Lawal, Bashir[c] ; Munyembaraga, Valens[d, e] ; Bakare, Oluwafemi Shittu[f] ; Taher, Muhammad[g, h] ; Khotib, Junaidi[i] ; Susanti, Deny[j] ; Oyinloye, Babatunji Emmanuel[b, k, l] ; Noriega, Lloyd[a] ; Famuti, Ayodeji[m] ; Fadaka, Adewale Oluwaseun[n] ; Ajiboye, Basiru Olaitan[l, o]

Save all to author list

[a] College of Medicine, Graduate Institute of Biomedical Sciences, China Medical University, Taichung, 40402, Taiwan
[b] Department of Chemical Sciences, Biochemistry Unit, Afe-Babalola University, Ekiti State, Ado-Ekiti, 360101, Nigeria
[c] Department of Pathology, University of Pittsburgh, Pittsburgh, 15213, PA, United States
[d] Institute of Translational Medicine and New Drug Development, College of Medicine, China Medical University, Taichung, 40402, Taiwan

View additional affiliations

View PDF Full text options Export

Abstract
Author keywords
Indexed keywords
Sustainable Development Goals 2023
SciVal Topics
Chemicals and CAS Registry Numbers

Abstract

Glucokinase plays an important role in regulating the blood glucose level and serves as an essential therapeutic target in type 2 diabetes management. Entada africana is a medicinal plant and highly rich source of bioactive ligands with the potency to develop new target drugs for glucokinase such as diabetes and obesity. Therefore, the study explored a computational approach to predict identified compounds from Entada africana following its intermolecular interactions with the allosteric binding site of the enzymes. We retrieved the three-dimensional (3D) crystal structure of glucokinase (PDB ID: 4L3Q) from the online protein data bank and prepared it using the Maestro 13.5, Schrödinger Suite 2022-3. The compounds identified were subjected to ADME, docking analysis, pharmacophore modeling, and molecular simulation. The results show the binding potential of the identified ligands to the amino acid residues, thereby suggesting an interaction of the amino acids with the ligand at the binding site of the glucokinase activator through conventional chemical bonds such as hydrogen bonds and hydrophobic interactions. The compatibility of the molecules was highly observed when compared with the standard ligand, thereby leading to structural and functional changes. Therefore, the bioactive components from Entada africana could be a good driver of glucokinase, thereby paving the way for the discovery of therapeutic drugs for the treatment of diabetes and its related complications. © 2023 by the authors.

Author keywords

Entada africana; glucokinase; hydrophobic; pharmacophore; simulation

Indexed keywords

Sustainable Development Goals 2023 New

SciVal Topics

Chemicals and CAS Registry Numbers

Metrics

Funding details

Funding sponsor	Funding number	Acronym
Ministry of Education, Culture, Research and Technology of the Republic of Indonesia		

Funding text

This research was funded by the Ministry of Education, Culture, Research and Technology of the Republic of Indonesia via Research Grant PDUPT for 2021–2022.

References (47)

View in search results format >

All

Export Print E-mail Save to PDF Create bibliography

1 Alam, S., Hasan, M.K., Neaz, S., Hussain, N., Hossain, M.F., Rahman, T.

Diabetes Mellitus: Insights from Epidemiology, Biochemistry, Risk Factors, Diagnosis, Complications and Comprehensive Management

(2021) *Diabetology*, 2 (2), pp. 36-50. Cited 47 times.
www.mdpi.com/journal/diabetology
doi: 10.3390/diabetology2020004

View at Publisher

2 Onikanni, A.S., Lawal, B., Olusola, A.O., Olugbodi, J.O., Sani, S., Ajiboye, B.O., Ilesanmi, O.B., (...), Wu, A.T.H.

Sterculia tragacantha Lindl Leaf Extract Ameliorates STZ-Induced Diabetes, Oxidative Stress, Inflammation and Neuronal Impairment

(2021) *Journal of Inflammation Research*, 14, pp. 6749-6764. Cited 15 times.
https://www.dovepress.com/getfile.php?fileID=76625
doi: 10.2147/JIR.S319673

View at Publisher

3 Association, A.D.
Introduction: Standards of medical care in diabetes—2022
(2022) *Am. Diabetes Assoc*, 45, pp. S1-S2. Cited 127 times.

4 Onikanni, S.A., Lawal, B., Oyinloye, B.E., Ajiboye, B.O., Ulziijargal, S., Wang, C.-H., Emran, T.B., (...), Simal-Gandara, J.

Mitochondrial defects in pancreatic beta-cell dysfunction and neurodegenerative diseases: Pathogenesis and therapeutic applications (Open Access)

(2023) *Life Sciences*, 312, art. no. 121247. Cited 2 times.
www.elsevier.com/locate/lifescie
doi: 10.1016/j.lfs.2022.121247

View at Publisher

5 Anyanwu, A., Olopade, O., Onung, S., Odeniyi, I., Coker, H., Fasanmade, O., Ohwovoriole, A.
Serum vitamin D levels in persons with type 2 diabetes mellitus in Lagos, Nigeria
(2020) *Int. J. Diabetes Clin. Res*, 7, p. 7. Cited 4 times.

6 Colomer, A., Igual, J., Naranjo, V.

Detection of early signs of diabetic retinopathy based on textural and morphological information in fundus images (Open Access)

(2020) *Sensors (Switzerland)*, 20 (4), art. no. 1005. Cited 54 times.
https://www.mdpi.com/1424-8220/20/4/1005/pdf
doi: 10.3390/s20041005

View at Publisher

7 Wang, H., Yuan, G., Zhao, X., Peng, L., Wang, Z., He, Y., Qu, C., (...), Peng, Z.

Hard exudate detection based on deep model learned information and multi-feature joint representation for diabetic retinopathy screening (Open Access)

(2020) *Computer Methods and Programs in Biomedicine*, 191, art. no. 105398. Cited 48 times.
www.elsevier.com/locate/cmpb
doi: 10.1016/j.cmpb.2020.105398

View at Publisher

8 Verhulst, M.J.L., Loos, B.G., Gerdes, V.E.A., Teeuw, W.J.

Evaluating all potential oral complications of diabetes mellitus (Open Access)

(2019) *Frontiers in Endocrinology*, 10 (FEB), art. no. 56. Cited 129 times.
https://www.frontiersin.org/journals/endocrinology#
doi: 10.3389/fendo.2019.00056

View at Publisher

9 Abdulrasheed-Adeleke, T., Lawal, B., Agwupuye, E.I., Kuo, Y., Eni, A.M., Ekoh, O.F., Lukman, H.Y., (...), Huang, H.-S.

Apigetrin-enriched Pulmeria alba extract prevents assault of STZ on pancreatic β-cells and neuronal oxidative stress with concomitant attenuation of tissue damage and suppression of inflammation in the brain of diabetic rats (Open Access)

(2023) *Biomedicine and Pharmacotherapy*, 162, art. no. 114582.
https://www.journals.elsevier.com/biomedicine-and-pharmacotherapy
doi: 10.1016/j.biopha.2023.114582

View at Publisher

10 Ajiboye, B.O., Oyinloye, B.E., Awurum, J.C., Onikanni, S.A., Adefolalu, A., Oluba, O.M.

Protective role of Sterculia tragacantha aqueous extract on pancreatic gene expression and oxidative stress parameters in streptozotocin-induced diabetic rats (Open Access)

(2022) *Journal of Complementary and Integrative Medicine*, 19 (2), pp. 317-327. Cited 3 times.
www.degruyter.com/view/j/jcim
doi: 10.1515/jcim-2021-0020

View at Publisher

11 Yang, W.-C.

Botanical, pharmacological, phytochemical, and toxicological aspects of the antidiabetic plant Bidens Pilosa L. (Open Access)

(2014) *Evidence-based Complementary and Alternative Medicine*, 2014, art. no. 698617. Cited 38 times.
doi: 10.1155/2014/698617

View at Publisher

12 Geck, M.S., Lecca, D., Marchese, G., Casu, L., Leonti, M.

Ethnomedicine and neuropsychopharmacology in Mesoamerica (Open Access)

(2021) *Journal of Ethnopharmacology*, 278, art. no. 114243. Cited 6 times.
www.elsevier.com/locate/jethpharm
doi: 10.1016/j.jep.2021.114243

View at Publisher

13 Xuan, T.D., Khanh, T.D.

Chemistry and pharmacology of Bidens pilosa: an overview (Open Access)

(2016) *Journal of Pharmaceutical Investigation*, 46 (2), pp. 91-132. Cited 59 times.
http://www.springer.com/biomed/journal/40005
doi: 10.1007/s40005-016-0231-6

View at Publisher

14 Ansari, P., Akther, S., Hannan, J.M.A., Seidel, V., Nujat, N.J., Abdel-Wahab, Y.H.A.

Pharmacologically Active Phytomolecules Isolated from Traditional Antidiabetic Plants and Their Therapeutic Role for the Management of Diabetes Mellitus (Open Access)

(2022) *Molecules*, 27 (13), art. no. 4278. Cited 23 times.
https://www.mdpi.com/1420-3049/27/13/4278/pdf?version=1656840801
doi: 10.3390/molecules27134278

View at Publisher

15 Yusuf, A.J., Abdullahi, M.I.
The phytochemical and pharmacological actions of Entada africana Guill. & Perr. (Open Access)

(2019) *Heliyon*, 5 (9), art. no. e02332. Cited 13 times.
http://www.journals.elsevier.com/heliyon/
doi: 10.1016/j.heliyon.2019.e02332

View at Publisher

16 Adewole, E., Yusuf, B., Ogola-Emma, E., Ojo, A., Adewumi, D.F., Oludoro, O., Akinwale, H., (...), Oyinloye, B.E.
PHYTOCHEMICALS PROFILE AND IN-VITRO ANTIDIABETIC POTENTIALS OF FRACTIONATED EXTRACTS OF ENTADA AFRICANA AND LEPTADENIA HASTATA (Open Access)

(2022) *ScienceRise: Pharmaceutical Science*, 2022 (3), pp. 65-73.
http://journals.uran.ua/sr_pharm/article/download/255744/256994
doi: 10.15587/2519-4852.2022.255744

View at Publisher

17 Semwal, D.K., Semwal, R.B., Combrinck, S., Viljoen, A.
Myricetin: A dietary molecule with diverse biological activities (Open Access)

(2016) *Nutrients*, 8 (2), art. no. 90. Cited 404 times.
http://www.mdpi.com/2072-6643/8/2/90/pdf
doi: 10.3390/nu8020090

View at Publisher

18 Salehi, B., Venditti, A., Sharifi-Rad, M., Kręgiel, D., Sharifi-Rad, J., Durazzo, A., Lucarini, M., (...), Martins, N.
The therapeutic potential of Apigenin (Open Access)

(2019) *International Journal of Molecular Sciences*, 20 (6), art. no. 1305. Cited 537 times.
https://www.mdpi.com/1422-0067/20/6/1305/pdf
doi: 10.3390/ijms20061305

View at Publisher

19 Sims, K.R., He, B., Koo, H., Benoit, D.S.W.
Electrostatic Interactions Enable Nanoparticle Delivery of the Flavonoid Myricetin (Open Access)

(2020) *ACS Omega*, 5 (22), pp. 12649-12659. Cited 20 times.
pubs.acs.org/journal/acsodf
doi: 10.1021/acsomega.9b04101

View at Publisher

20 Rahman, A.-U.
Studies in Natural Products Chemistry
(2023) *Studies in Natural Products Chemistry*, 76, p. 2.
Elsevier, Amsterdam, The Netherlands

21 Umar, H.I., Josiah, S.S., Saliu, T.P., Jimoh, T.O., Ajayi, A., Danjuma, J.B.
In-silico analysis of the inhibition of the SARS-CoV-2 main protease by some active compounds from selected African plants (Open Access)

(2021) *Journal of Taibah University Medical Sciences*, 16 (2), pp. 162-176. Cited 25 times.
http://www.elsevier.com/journals/journal-of-taibah-university-medical-sciences/1658-3612
doi: 10.1016/j.jtumed.2020.12.005

View at Publisher

22 Romano, J.D., Tatonetti, N.P.

Informatics and computational methods in natural product drug discovery: A review and perspectives (Open Access)

(2019) *Frontiers in Genetics*, 10 (APR), art. no. 368. Cited 76 times.
https://www.frontiersin.org/journals/genetics#
doi: 10.3389/fgene.2019.00368

View at Publisher

23 Zainab, B., Ayaz, Z., Alwahibi, M.S., Khan, S., Rizwana, H., Soliman, D.W., Alawaad, A., (...), Mehmood Abbasi, A.

In-silico elucidation of Moringa oleifera phytochemicals against diabetes mellitus (Open Access)

(2020) *Saudi Journal of Biological Sciences*, 27 (9), pp. 2299-2307. Cited 28 times.
http://www.ksu.edu.sa/sites/Colleges/CollegeofScinces/BotanyDepartment/SJBS/Default.aspx
doi: 10.1016/j.sjbs.2020.04.002

View at Publisher

24 Shahrajabian, M.H., Sun, W., Cheng, Q.

The Importance of Flavonoids and Phytochemicals of Medicinal Plants with Antiviral Activities (Open Access)

(2022) *Mini-Reviews in Organic Chemistry*, 19 (3), pp. 293-318. Cited 16 times.
http://www.eurekaselect.com/issue/11204
doi: 10.2174/1570178618666210707161025

View at Publisher

25 Ajiboye, B.O., Iwaloye, O., Owolabi, O.V., Ejeje, J.N., Okerewa, A., Johnson, O.O., Udebor, A.E., (...), Oyinloye, B.E.

Screening of potential antidiabetic phytochemicals from Gongronema latifolium leaf against therapeutic targets of type 2 diabetes mellitus: multi-targets drug design

(2022) *SN Applied Sciences*, 4 (1), art. no. 14. Cited 6 times.
springer.com/snas
doi: 10.1007/s42452-021-04880-2

View at Publisher

26 Oyinloye, B.E., Iwaloye, O., Ajiboye, B.O.

Polypharmacology of Gongronema latifolium leaf secondary metabolites against protein kinases implicated in Parkinson's disease and Alzheimer's disease (Open Access)

(2021) *Scientific African*, 12, art. no. e00826. Cited 13 times.
https://www.journals.elsevier.com/scientific-african
doi: 10.1016/j.sciaf.2021.e00826

View at Publisher

27 Mekhilef, S., Saidur, R., Kamalisarvestani, M.

Effect of dust, humidity and air velocity on efficiency of photovoltaic cells (Open Access)

(2012) *Renewable and Sustainable Energy Reviews*, 16 (5), pp. 2920-2925. Cited 475 times.
doi: 10.1016/j.rser.2012.02.012

View at Publisher

28 Kaushik, A., Kaushik, M.

Recent updates on glucokinase activators and glucokinase regulatory protein disrupters for the treatment of type 2 diabetes mellitus (Open Access)

(2019) *Current Diabetes Reviews*, 15 (3), pp. 205-212. Cited 4 times.
http://www.eurekaselect.com/164011
doi: 10.2174/1573399814666180724100749

View at Publisher

29 Wang, H., Tian, Q., Zhang, J., Liu, H., Zhang, J., Cao, W., Zhang, X., (...), Wang, Y.

Blood transcriptome profiling as potential biomarkers of suboptimal health status: potential utility of novel biomarkers for predictive, preventive, and personalized medicine strategy (Open Access)

(2021) *EPMA Journal*, 12 (2), pp. 103-115. Cited 7 times.
http://www.springer.com/journal/13167/about
doi: 10.1007/s13167-021-00238-1

View at Publisher

30 Chavda, V.P., Ajabiya, J., Teli, D., Bojarska, J., Apostolopoulos, V.

Tirzepatide, a New Era of Dual-Targeted Treatment for Diabetes and Obesity: A Mini-Review (Open Access)

(2022) *Molecules*, 27 (13), art. no. 4315. Cited 35 times.
https://www.mdpi.com/1420-3049/27/13/4315/pdf?version=1657082233
doi: 10.3390/molecules27134315

View at Publisher

31 Chung, M.-Y., Choi, H.-K., Hwang, J.-T.

Ampk activity: A primary target for diabetes prevention with therapeutic phytochemicals

(2021) *Nutrients*, 13 (11), art. no. 4050. Cited 14 times.
https://www.mdpi.com/2072-6643/13/11/4050/pdf
doi: 10.3390/nu13114050

View at Publisher

32 Mashau, M.E., Ramatsetse, K.E., Ramashia, S.E.

Effects of adding moringa oleifera leaves powder on the nutritional properties, lipid oxidation and microbial growth in ground beef during cold storage

(2021) *Applied Sciences (Switzerland)*, 11 (7), art. no. 2944. Cited 15 times.
https://www.mdpi.com/2076-3417/11/7/2944/pdf
doi: 10.3390/app11072944

View at Publisher

33 Ajiboye, B.O., Fagbola, T.M., Folorunso, I.M., Salami, A.W., Aletile, O.N., Akomolede, B.A., Ayemoni, F.I., (...), Oyinloye, B.E.

In silico identification of chemical compounds in Spondias mombin targeting aldose reductase and glycogen synthase kinase 3β to abate diabetes mellitus (Open Access)

(2023) *Informatics in Medicine Unlocked*, 36, art. no. 101126.
http://www.journals.elsevier.com/informatics-in-medicine-unlocked
doi: 10.1016/j.imu.2022.101126

View at Publisher

34 Tibiri, A., Rakotonandrasana, O., Nacoulma, G.O., Banzouzi, J.T.

Radical scavenging activity, phenolic content and cytotoxicity of bark and leaves extracts of Entada africana Guill. and Perr. (Mimosaceae) (Open Access)

(2007) *Journal of Biological Sciences*, 7 (6), pp. 959-963. Cited 13 times.
http://scialert.net/current.php?issn=1727-3048
doi: 10.3923/jbs.2007.959.963

View at Publisher

35 Obakiro, S.B., Kiprop, A., Kigondu, E., K'owino, I., Kiyimba, K., Drago Kato, C., Gavamukulya, Y.

Sub-Acute Toxicity Effects of Methanolic Stem Bark Extract of Entada abyssinica on Biochemical, Haematological and Histopathological Parameters in Wistar Albino Rats (Open Access)

(2021) *Frontiers in Pharmacology*, 12, art. no. 740305. Cited 8 times.
http://www.frontiersin.org/Pharmacology
doi: 10.3389/fphar.2021.740305

View at Publisher

36 Kouam, A.F., Owona, B.A., Fifen, R., Njayou, F.N., Moundipa, P.F.

Inhibition of CYP2E1 and activation of Nrf2 signaling pathways by a fraction from Entada africana alleviate carbon tetrachloride-induced hepatotoxicity (Open Access)

(2020) *Heliyon*, 6 (8), art. no. e04602. Cited 9 times.
http://www.journals.elsevier.com/heliyon/
doi: 10.1016/j.heliyon.2020.e04602

View at Publisher

37 Tiwari, G., Mohanty, D.

An In Silico Analysis of the Binding Modes and Binding Affinities of Small Molecule Modulators of PDZ-Peptide Interactions

(2013) *PLoS ONE*, 8 (8), art. no. e71340. Cited 18 times.
http://www.plosone.org/article/fetchObjectAttachment.action;jsessionid=D3145D5A9DA440B78145B2EEFECBAAD8?uri=info%3Adoi%2F10.1371%2Fjournal.pone.0071340&representation=PDF
doi: 10.1371/journal.pone.0071340

View at Publisher

38 Tao, X., Huang, Y., Wang, C., Chen, F., Yang, L., Ling, L., Che, Z., (...), Chen, X.

Recent developments in molecular docking technology applied in food science: a review

(2020) *International Journal of Food Science and Technology*, 55 (1), pp. 33-45. Cited 86 times.
http://onlinelibrary.wiley.com/journal/10.1111/(ISSN)1365-2621
doi: 10.1111/ijfs.14325

View at Publisher

39 Onikanni, S.A., Lawal, B., Fadaka, A.O., Bakare, O., Adewole, E., Taher, M., Khotib, J., (...), Sibuyi, N.R.S.

Computational and Preclinical Prediction of the Antimicrobial Properties of an Agent Isolated from Monodora myristica: A Novel DNA Gyrase Inhibitor (Open Access)

(2023) *Molecules*, 28 (4), art. no. 1593. Cited 2 times.
http://www.mdpi.com/journal/molecules
doi: 10.3390/molecules28041593

View at Publisher

40 Borkotoky, S., Banerjee, M.

A computational prediction of SARS-CoV-2 structural protein inhibitors from Azadirachta indica (Neem) (Open Access)

(2021) *Journal of Biomolecular Structure and Dynamics*, 39 (11), pp. 4111-4121. Cited 66 times.
http://www.tandfonline.com/loi/tbsd20
doi: 10.1080/07391102.2020.1774419

View at Publisher

41 Genheden, S., Kuhn, O., Mikulskis, P., Hoffmann, D., Ryde, U.

The normal-mode entropy in the MM/GBSA method: Effect of system truncation, buffer region, and dielectric constant (Open Access)

(2012) *Journal of Chemical Information and Modeling*, 52 (8), pp. 2079-2088. Cited 138 times.
http://pubs.acs.org/journal/jcisd8
doi: 10.1021/ci3001919

View at Publisher

42 Forouzesh, N., Mishra, N.

An effective MM/GBSA protocol for absolute binding free energy calculations: A case study on SARS-CoV-2 spike protein and the human ACE2 receptor (Open Access)

(2021) *Molecules*, 26 (8), art. no. 2383. Cited 33 times.
http://www.mdpi.com/journal/molecules
doi: 10.3390/molecules26082383

View at Publisher

43 Ekins, S., Mestres, J., Testa, B.

In silico pharmacology for drug discovery: Methods for virtual ligand screening and profiling (Open Access)

(2007) *British Journal of Pharmacology*, 152 (1), pp. 9-20. Cited 469 times.
doi: 10.1038/sj.bjp.0707305

View at Publisher

44 Adewole, E., Ogola-Emma, E., Ojo, A., Adegbite, S.

GC-MS Compound Identification in Phaseolus vulgaris-A Low-Cost Cataract Prevention Food

(2022) *Food Science and Technology (United States)*, 10 (3), pp. 112-119.
https://www.hrpub.org/download/20220830/FST4-11126885.pdf
doi: 10.13189/fst.2022.100304

View at Publisher

45 Johnson, T.O., Adegboyega, A.E., Iwaloye, O., Eseola, O.A., Plass, W., Afolabi, B., Rotimi, D., (...), Adeyemi, O.S.

Computational study of the therapeutic potentials of a new series of imidazole derivatives against SARS-CoV-2 (Open Access)

(2021) *Journal of Pharmacological Sciences*, 147 (1), pp. 62-71. Cited 22 times.
http://www.jstage.jst.go.jp/browse/
doi: 10.1016/j.jphs.2021.05.004

View at Publisher

46 Oselusi, S.O., Fadaka, A.O., Wyckoff, G.J., Egieyeh, S.A.

Computational Target-Based Screening of Anti-MRSA Natural Products Reveals Potential Multitarget Mechanisms of Action through Peptidoglycan Synthesis Proteins (Open Access)

(2022) *ACS Omega*, 7 (42), pp. 37896-37906. Cited 4 times.
pubs.acs.org/journal/acsodf
doi: 10.1021/acsomega.2c05061

View at Publisher

47 Adekiya, T.A., Aruleba, R.T., Klein, A., Fadaka, A.O.

In silico inhibition of SGTP4 as a therapeutic target for the treatment of schistosomiasis (Open Access)

(2022) *Journal of Biomolecular Structure and Dynamics*, 40 (8), pp. 3697-3705. Cited 9 times.
http://www.tandfonline.com/loi/tbsd20
doi: 10.1080/07391102.2020.1850363

View at Publisher

Onikanni, S.A.; College of Medicine, Graduate Institute of Biomedical Sciences, China Medical University, Taichung, Taiwan; email:u109305123@cmu.edu.tw
Khotib, J.; Department of Pharmacy Practice, Faculty of Pharmacy, Airlangga University, Surabaya, Indonesia; email:junaidi-k@ff.unair.ac.id

About Scopus

What is Scopus

Content coverage

Scopus blog

Scopus API

Privacy matters

Language

日本語版を表示する

查看简体中文版本

查看繁體中文版本

Просмотр версии на русском языке

Customer Service

Help

Tutorials

Contact us