



Abstract Pharmacological Network Study on the Effect of Quercetin on Gastric Cancer Using Computerized Databases [†]

Sergio Raúl Zúñiga-Hernández ^{1,*}, Trinidad García-Iglesias ², Monserrat Macías-Carballo ³, Juan Manuel Guzmán-Flores ⁴ and Christian Martin Rodríguez-Razón ⁵

- ¹ Centro Universitario de Los Altos, Doctorado en biociencias, Universidad de Guadalajara, Tepatitlán de Morelos 47620, Mexico
- ² Departamento de Fisiología del Centro Universitario de las Ciencias de la Salud, INICIA Instituto de Investigación de Cáncer en la Infancia y Adolescencia, Guadalajara 44340, Mexico; trinidad.giglesias@academicos.udg.mx
- ³ Instituto de Investigación en Ciencias Médicas, Centro Universitario de Los Altos, Universidad de Guadalajara, Tepatitlán de Morelos 47620, Mexico; monserrat.macias@cualtos.udg.mx
- ⁴ Instituto de Investigación en Biociencias, Centro Universitario de Los Altos, Universidad de Guadalajara, Tepatitlánn de Morelos 47620, Mexico; jmanuel.guzman@academicos.udg.mx
- ⁵ Laboratorio de Experimentación Animal (Bioterio), Departamento de Ciencias de la Salud, Centro Universitario de Los Altos, Tepatitlán de Morelos 47620, Mexico; christian.rrazon@academicos.udg.mx
- * Correspondence: sergio.zuniga@alumnos.udg.mx
- [†] Presented at the 4th International Electronic Conference on Cancers, 6–8 March 2024; Available online: https://sciforum.net/event/IECC2024.

Abstract: Gastric cancer (GC) is the second most common cause of death of any cancer-related cases in the world, and is also in the top 5 most common malignancy cancers in general. There are plenty of welldistributed treatments, offering better hygiene, more robust and complete nutrition, and the eradication of pathogens such as Helicobacter pylori. Currently, there is still the need for more treatments, especially those of lower cost, like those coming from already easily available products. Quercetin (QRC) is a natural phenolic compound present in a wide variety of products, e.g., in plants like Hibiscus sabdariffa, onions, grapes, broccoli, and citrus fruits. This product has been shown to have great potential therapeutic effects, and it has also been suggested that it could be useful in combating different types of cancer; however, information regarding the targets or mechanisms that QRC has on cancer cells is still unclear. Therefore, this study aims to identify the targets that QRC has, like anti-cancer treatment for GC using different bioinformatic tools and databases. From MalaCards and SwissTargetPrediction, both QRC and GC molecular targets were defined, and then they were matched with the Venny 2.1.0 platform. From this, 31 genes were gathered, and then they were analyzed using the ShinnyGo0.77 and DAVID-Bioinformatic Resources. Furthermore, StringDB was used to identify the protein-protein interactions, and Citoscape 3.6.0 12 hub genes were obtained. Those hub genes were then subject to Gene Expression Profiling Interactive Analysis and TISIDB. Finally, molecular docking studies were performed using the SwissDock database. The results suggest that, according to the gene ontology data, QRC has a relationship with the regulation of cell death, response to stress, cell motility, response to amyloid-beta, cellular response to reactive oxygen species, and apoptotic processes. Some genes like EGFR were correlated with an abundance of CD8 and Neutrophil infiltration but didn't show to improve the survival rate. Furthermore, molecular docking results show that QRC can bind to multiple molecules of interest. These results complement some of the currently available information alluding to the effectiveness of plants rich with QRC as part of the treatment used for different kinds of cancer, but it also suggests a plethora of new targets that this molecule has in GC, while at the same time giving a clearer idea of the mechanisms that are affected in GC by QRC. However, as with any other study that primarily uses bioinformatic tools, these final results are to be used for more direct and precise research, especially if experimental protocols are used.

Keywords: quercetin; network; gastric cancer; bioinformatics



Citation: Zúñiga-Hernández, S.R.; García-Iglesias, T.; Macías-Carballo, M.; Guzmán-Flores, J.M.; Rodríguez-Razón, C.M. Pharmacological Network Study on the Effect of Quercetin on Gastric Cancer Using Computerized Databases. *Proceedings* **2024**, *100*, 10. https://doi.org/10.3390/ proceedings2024100010

Academic Editor: Ulrich Pfeffer

Published: 27 March 2024



Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). **Supplementary Materials:** The following are available online at https://www.mdpi.com/article/ 10.3390/proceedings2024100010/s1.

Author Contributions: Conceptualization, S.R.Z.-H. and C.M.R.-R.; methodology, J.M.G.-F.; software, J.M.G.-F.; validation, J.M.G.-F., S.R.Z.-H. and M.M.-C.; formal analysis, S.R.Z.-H.; investigation, T.G.-I.; resources, C.M.R.-R.; data curation, C.M.R.-R.; writing—original draft preparation, S.R.Z.-H.; writing—review and editing, S.R.Z.-H.; visualization, T.G.-I.; supervision, C.M.R.-R.; project administration, M.M.-C.; funding acquisition, C.M.R.-R. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Venny 2.1: (https://bioinfogp.cnb.csic.es/tools/venny/ accessed on 26 March 2024) accessed on 26 March 2024 Swiss Target Prediction (http://www.swisstargetprediction. ch/ accessed on 26 March 2024), Malacards (https://www.malacards.org/ accessed on 26 March 2024), ShinnyGo 0.8 site (http://bioinformatics.sdstate.edu/go/ accessed on 26 March 2024), StringDB site (https://string-db.org/ accessed on 26 March 2024), GEPIA2 (http://gepia2.cancer-pku.cn/#index accessed on 26 March 2024), TISIDB website (http://cis.hku.hk/TISIDB/ accessed on 26 March 2024), SwissDock (http://www.swissdock.ch/ accessed on 26 March 2024) and UCSF CHIMERA (https://www.cgl.ucsf.edu/chimera/docs/ContributedSoftware/webdata/webdata.html#browser accessed on 26 March 2024).

Conflicts of Interest: The authors declare no conflict of interest.

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.