Commentary
Volume 12:6, 2022

Medicinal Chemistry

ISSN: 2161-0444 Open Access

Molecular Docking Study, Therapeutic Potential and Botanical Sources

Amelia Ann*

Department of Molecular Medicine, Aston University, Aston St, Birmingham, UK

Description

Alternative medicine and natural remedies are becoming more and more well-liked for the treatment of illnesses like cancer, hepatic, cardiovascular, and neurological disorders. It has been proven that flavonoids, the natural polyphenolic components that are typically found in the foods we eat on a daily basis, can be used to treat or manage various types of illnesses. Agathisflavone, also known as 8-[5,7-dihydroxy-2 (4-hydroxyphenyl)-4-oxochromen-6-yl] ($C_{30}H_{18}O_{10}$ chemical formula) A biflavonoid produced from plants called 5,7-dihydroxy-2-(4 hydroxyphenyl)chromen-4-one (MW: 538.464 g/mol) has gained attention for its wide range of biological functions. In pluripotent stem (miPS) cells, agathisflavone at 60 M with/without 2 M retinoic acid increased neurogenesis and the expression of retinoic acid receptors and. Additionally, this bioflavone induced neuroinflammation and decreased neurotoxicity in BV2 microglia and SH-SY5Y cells *via* the SIRT1 related pathway. Additionally, it has been claimed to have neuroprotective properties that may be mediated through rat primary cortical neurons' GABAA (gamma-aminobutyric acid) subunit receptors. It was found that the GABAA-benzodiazepine receptor interacted and had modulatory effects. Additionally, this bioflavone had neuroprotective effects in the cerebral hemispheres of Wistar rats by inhibiting antagonists of oestrogen receptors (ER and ER), decreasing the expression of TNF-, IL-1, and IL-6, and increasing the expression of IL-10, arginase 1, and neuroprotective trophic factors like brain-derived neurotrophic factor (BDNF), nerve growth factor, and others (NGF) [1].

The 17 therapeutically significant biomacromolecules TNF-, iNOS, COX-2, NF-B, IL-1, IL-6, IL-10, arginase 1, GABAA, BDNF, NGF, NT4, GDNF, EAAT1, and SGPT were the targets of the molecular docking investigation with agathisflavone. Using Modeller, homology models of these crucial proteins were created using the Protein Data Bank (PDB) published models as templates. The binding sites in these proteins were predicted using the ProBiS service, and the ligand, agathisflavone, was synthesised using AutoDockTools. The active binding site was encircled by an initial docking grid of 40 40 40 and 0.8, and the synthesised ligand was docked using AutoDock Vina into the anticipated binding pocket of the chosen proteins. In pluripotent stem (miPS) cells, agathisflavone at 60 M with/without 2 M retinoic acid increased neurogenesis and the expression of retinoic acid receptors and. Additionally, this bioflavone induced neuroinflammation and decreased neurotoxicity in BV2 microglia and SH-SY5Y cells via the SIRT1 related pathway. Additionally, it has been claimed to have neuroprotective properties that may be mediated through rat primary cortical neurons' GABAA (gamma-aminobutyric acid) subunit receptors. It was found that the GABAA-benzodiazepine receptor interacted and had modulatory effects [2,3].

Reactive oxygen species (ROS) do, however, have a number of beneficial functions, but their overproduction can have negative impacts on human health. For instance, OH is one of the most dangerous and short-lived free radicals in our body (biological half-life (t1/2): 109 s). It is clear that it has negative biological consequences on human bodies, including lipid peroxidation. Fenton was the first to notice that Cu^{2+} or Fe^{2+} reacting with hydrogen peroxide (H_2O_2) results in OH. On the other hand, NO is produced naturally in activated macrophages and endothelial cells, and it is thought to have a role in a number of illnesses based on organ reperfusion and inflammation. This includes atherosclerosis and cancer. According to physiological concentrations, it is a slow reactive nitrogen species (RNS).Through interactions with the active metal phases, the method's efficiency is primarily influenced by the support's surface characteristics. According to reports, the aligned nanotubes grow on a matrix with a highly homogenous distribution of transition metal thanks to the sol-gel manufacturing technique. To make the process reproducible, the supported-catalyst activity must be carefully managed because every applied condition has an impact on it. In addition to the preparation process, the metal-to-support content ratio affects how metal particles are dispersed on the support. The catalyst and support have an ideal metal content ratio, which results in the synthesis of CNTs with the appropriate characteristics [4,5].

***Address for Correspondence:** Amelia Ann, Department of Molecular Medicine, Aston University, Aston St, Birmingham, UK; E-mail:ann.amelia@ac.za*

Date of Submission: 03 June, 2022, Manuscript No. MCCR-22-70476; **Editor Assigned:** 05 June, 2022, PreQC No. P-70476; **Reviewed:** 10 June, 2022, QC No. Q-70476; **Revised:** 15 June, 2022, Manuscript No. R-70476; **Published:** 20 June, 2022, DOI: 10.37421/2161-0444.2022.12.628

Acknowledgement

None.

Conflict of Interest

The author reported no potential conflict of interest.

References

1. Ogungbe, Ifedayo Victor and William N. Setzer. "The potential of secondary metabolites from plants as drugs or leads against protozoan neglected diseases-(Part III): *In-silico* molecular docking investigations." *Mol* 21 (2016): 1389.
2. Rodríguez, David, Anirudh Ranganathan and Jens Carlsson. "Discovery of GPCR ligands by molecular docking screening: Novel opportunities provided by crystal structures." *Cur Topics Med Chem* 15 (2015): 2484-2503.
3. Gomha, Sobhi M., Zeinab A. Muhammad, Elham Ezz El-Arab and Islam K. Matar, et al. "Design, synthesis, molecular docking study and anti-hepatocellular carcinoma evaluation of new bis-triazolothiadiazines." *Mini Rev Med Chem* 20 (2020): 788-800.
4. Tu, Mengchen, Xin Zheng, Peiyuan Liu and Xinyu Liu, et al. "Typical organic pollutant-protein interactions studies through spectroscopy, molecular docking and crystallography: A review." *Sci Tot Env* 763 (2021): 142959.
5. Kumar, D. Thirumal and C. George Priya Doss. "Investigating the inhibitory effect of wortmannin in the hotspot mutation at codon 1047 of PIK3CA kinase domain: A molecular docking and molecular dynamics approach." *Adv Protein Chem Struc Bio* 102 (2016): 267-297.

How to cite this article: Ann, Amelia. "Molecular Docking Study, Therapeutic Potential and Botanical Sources." Med Chem 12 (2022): 628.