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PASS: Prediction of Activity Spectra for Biologically Active Constituent of Isoquercetin

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Research Article

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ABSTRACT

The PASS online prediction tool is effectively utilized for predicting the activity spectra of substances, relying on the 2D structures of biologically active compounds. In this study, observed that Pass prediction of active compound of isoquercetin show that maximum activity against membrane integrity agonist. This active compound of isoquercetin agent that promotes the maintenance, restoration, or strengthening of cell membrane integrity.

Keywords: Pass, Spectra, Active Constituent, Isoquercetin, flavonoids

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1. INTRODUCTION

Isoquercetin is the main component of Annona squamosa leaves for its antidiabetic and antioxidative effects (Panda and Kar, 2007). Recent investigation was made to reveal the involvement of a quercetin in the antidiabetic and antiperoxidative effects of Annona squamosa leaf extract. Quercetin-3-O-glucoside (characterized by UV, IR, MS and NMR analyses) was isolated from Annona squamosa leaves and examined for its potential to regulate alloxan-induced hyperglycemia and lipid peroxidation (LPO) in rats (Sunanda Panda, Anand Kar (2008). Isoquercetin's structure consists of the quercetin flavonoid molecule with a beta-D-glucopyranoside (a sugar) attached to the third carbon (C3) position. This means it is a quercetin-3-O-β-D-glucoside. The quercetin part has a three-ring structure with hydroxyl groups and a carbonyl group, while the attached glucose forms a ring structure, linking via an oxygen atom at the C3 of quercetin.

PASS Online predicts over 4000 kinds of biological activity, including pharmacological effects, mechanisms of action, toxic and adverse effects, interaction with metabolic enzymes and transporters, influence on gene expression, etc. To obtain the predicted biological activity profile for your compound, only structural formula is necessary; thus, prediction is possible even for virtual structure designed in computer but not synthesized yet. Aim of the present study was Prediction of activity Spectra for biologically active constituent of Isoquercetin through web server of way 2drug.

2.MATERIALS AND METHODS

Isoquercetin is the main component of *Annona squamosa* leaves for its antidiabetic and antioxidative effects (Panda and Kar, 2007). The Internet version of the program, PASS Inet predicted active constituents of Polygodial were send via the Internet a standard Molfile, which was prepared with the ISIS/Draw chemical editor website on http://www.mdli.com. The biological activity spectrum of PASS was designed and prediction was made with the comparison from the source data available https://way2drug.com/PassOnline/predict.php. Biological activity spectrum of a compound presents exhibit its activity despite the difference in essential conditions of its experimental determination. PASS outcomes are revealed by Pa (probability for active molecule) and Pi (probability for inactive molecule) scores. Having potentialities, the Pa and Pi scores vary in the range 0.00–1.00; usually, Pa + Pi ≠ 1, as these potentialities are predicted freely.
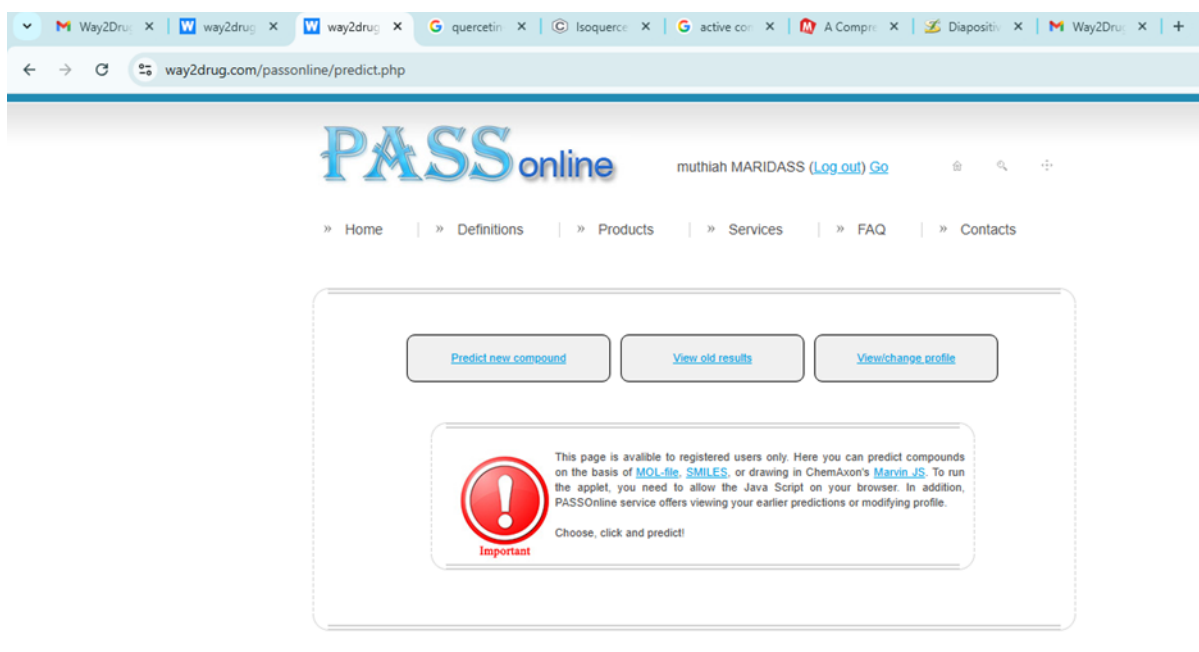

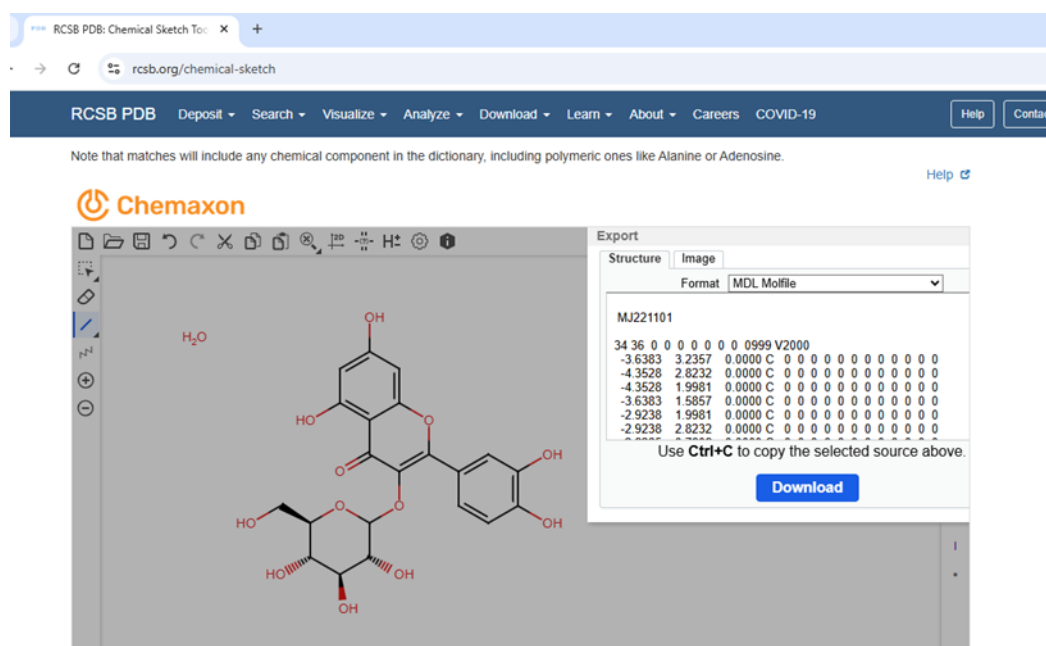Fig.1: PASS: Prediction website

Fig.2: Draw the structure of Isoquercetin and MDL mole file through online CHEM Draw software
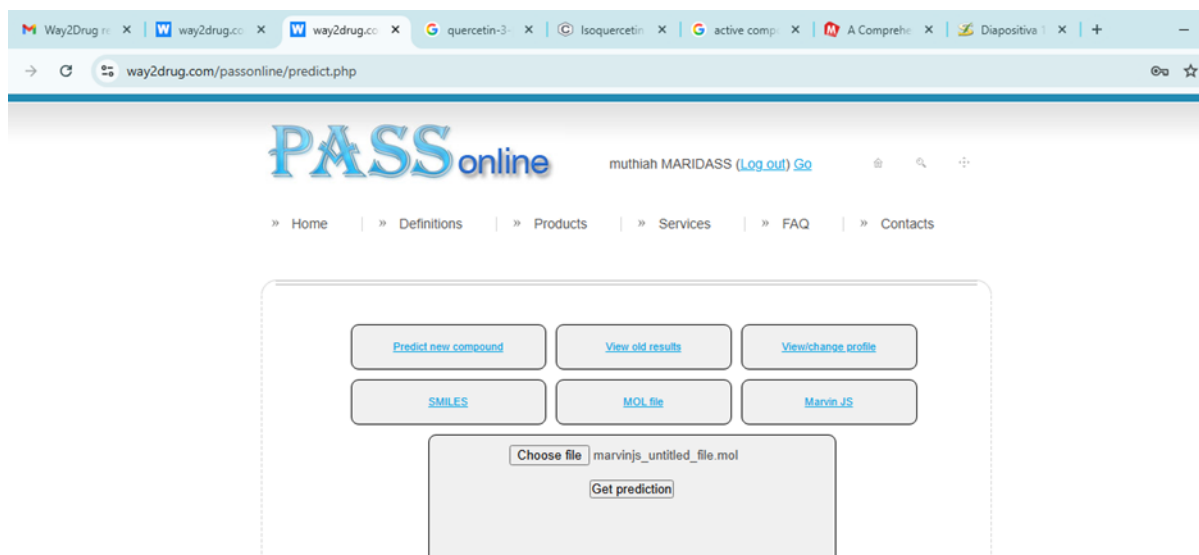
Fig.3: Pass Prediction of Isoquercetin and MDL mole file through online CHEM Draw software

3.RESULTS AND DISCUSSION

The results showed that Isoquercetin could possess several biological activities including Heptoprotectant (through the server https://way2drug.com/PassOnline/predict.php,(Table-1). In the present study, Isoquercetin's structure features a quercetin aglycone with a glucose sugar attached to the 3-position of the flavonoid's C ring, forming a chain-like glycoside linkage. Specifically, it is a quercetin-3-O-β-D-glucoside, a molecule composed of the aglycone quercetin (a pentahydroxyflavone) and a glucose moiety linked via a β-glycosidic bond. This glucose unit is attached through a C-O-C linkage, forming the "chain" that distinguishes isoquercetin from its aglycone, quercetin. Initially, biological activities of partially acylated esters were predicted using the PASS web tool. The prediction of spectrum biological activities was performed by applying the PASS web server. The PASS results are quoted as Pa and Pi and are displayed in Table 1. It was manifest from Table 1 that isoquercetin showed $0.989 < Pa < 0.001$ for membrane integrity agonist, $0.987 < Pa < 0.001$ for haemostatic, and other activities.

Table-1: Results of the pass prediction of biological activities of Isoquercetin

Pa	Pi	Activity
0,989	0,001	Membrane integrity agonist
0,987	0,001	Hemostatic
0,984	0,001	Cardioprotectant
0,983	0,001	Monophenol monooxygenase inhibitor
0,981	0,001	Membrane permeability inhibitor
0,978	0,001	Free radical scavenger
0,976	0,002	Lipid peroxidase inhibitor
0,965	0,001	Anticarcinogenic
0,961	0,000	Beta-N-acetylhexosaminidase inhibitor
0,961	0,001	Hepatoprotectant

4. CONCLUSION

Conclusion of the present study observed that Pass prediction of Isoquercetin show that maximum activity against membrane integrity agonist. This active compound of Isoquercetin agent that promotes the maintenance, restoration, or strengthening of cell membrane integrity.

5. ACKNOWLEDGEMENTS

6. CONFLICT OF INTEREST

None.

7. REFERENCES

Sunanda Panda, and Anand Kar (2008). Antidiabetic and antioxidative effects of Annona squamosa leaves are possibly mediated through quercetin-3-O-glucoside, BioFactors, https://doi.org/10.1002/biof.5520310307.