INTERNATIONAL JOURNAL OF ADVANCE RESEARCH, IDEAS AND INNOVATIONS IN TECHNOLOGY

ISSN: 2454-132X

Impact factor: 4.295

(Volume3, Issue1)

Available online at: www.ijariit.com

Identify the Bioactivity of Flavonoids in Erythrina Varigata Leaves Extracts Using the Pass Method

Geetha .S
Assistant Professor
Dept. of Chemistry
Jaya College of Arts & Science
Thiruvallur, India.
geethamar492@gmail.com

Dr. S. R. Divya
Visiting Professor
Dept. of Biochemistry
Jaya College of Arts & Science
Thiruvallur, India.
palsdivya@gmail.com

Dr. A. Chandramohan*
Associate Professor
Dept. of Biochemistry
Jaya College of Arts & Science
Thiruvallur, India.
chandru2c813@gmail.com

ABSTRACT - Erythrina Varigata plant as revealed from various literature resources, our work will planned to predict the bioactivity of Erythrina Varigata leave extracts using the 'PASS' software. The PASS predictions for the bioactivity of the sixteen flavonoids were found to be in the ranges from 65 to 97.7% as various inhibitors. Among the sixteen flavonoids from Erythrina Varigata leave, Vogelin – A and Isowigteone were found to exhibit more bioactivity like Monophenol monooxygenase inhibitor (96.3, 97.7%), Membrane integrity agonist (91.4, 92.6%), CYP1A inhibitor (95.2, 95.3%), CYP1A1 inhibitor (95.7%), MMP9 expression inhibitor (89.8, 90.6%), Histidine kinase inhibitor (93.7, 94.4%), UGT1A10 substrate (92.4, 95.3%), Chalcone isomerase inhibitor (93.1, 93.0%), Aldehyde oxidase inhibitor (91.3, 89.4%), CYP1A substrate (89.1%).

Keywords - PASS, Flavonoids, Erythrina Varigata, CYP1A inhibitor.

I. INTRODUCTION

Erythrina varigata plant is a traditional medicine system [1, 2]. Many people still use traditional herbs to treat a variety of diseases including bacterial infection [3, 4]. The development of resistance by pathogens to many of the commonly used antibiotics provides sufficient impetus for further attempts to search for new antimicrobial agent [5] and investigate the antimicrobial activity of Erythrina varigata plant [6, 10]. Flavonoids are beneficial for our health, because they often work as antioxidants in our body. The flavonoids in Erythrina varigata leave include many different compounds, such as flavonols, flavones, isoflavones, catechines and anthocyanidins [11]. Knowing the various bio-activities of flavonoids present in Erythrina Varigata and continuation of our work in determining the binding energy to predict the stability of flavonoids by computational chemistry our present work on the bioactivity using PASS software. Pa and Pi values were found to be estimate the chance that the studied compound is belonging to the sub-class of active and inactive compounds to resemble the structure of molecules and the most typical in a sub-set of actives and inactives in PASS training sets [12 – 14].

II. Structure

The original molecular structures of all the flavonoids were drawn in molinspiration online software.

Fig 1: Pterocarpan Group -I

Fig 2: Pterocarpan Group -II

Fig 3: Isowigteone

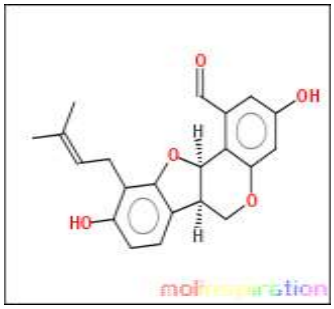

Fig 4: 1-Methoxyphaseolludin

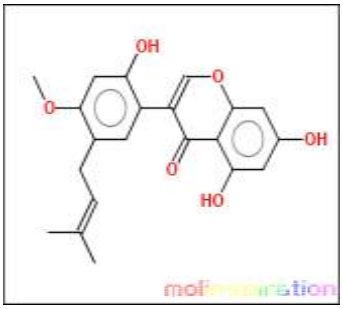

Fig 5: Vogelin- A

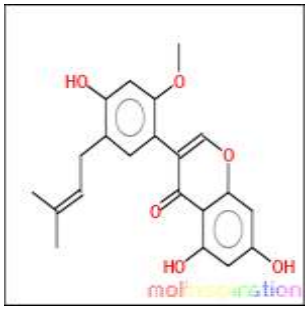

Fig 6: Vogelin-B

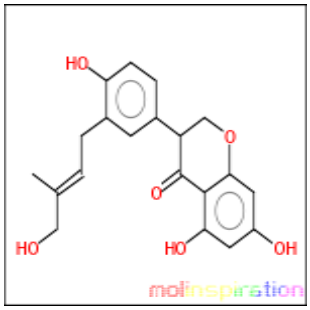

Fig 7: Vogelin- E

Fig 8: Vogelin- F

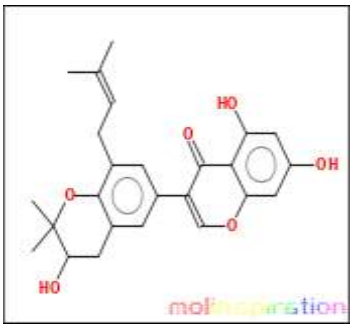

Fig 9: Vogelin –G

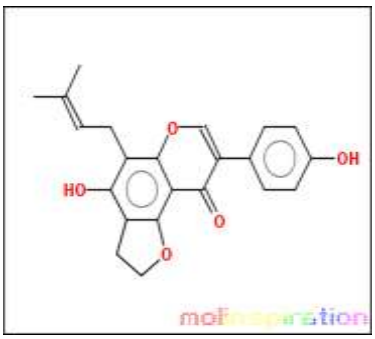

Fig 10: Vogelin- H

Fig 11: Vogelin-I

Fig 12: Vogelin-J

Fig 13: Erysenegalensin-G

Fig 14: Erysenegalensin- L

Fig 15: Erysenegalensin-M

Fig 16: Erysenegalensin-F

Table-1a: PASS prediction activity of flavonoids

S.No	Name of activity	Name of the flavonoids	PASS values (>65-90%) P_a/P_i	
			P_a	P_i
1	Membrane integrity agonist	Isowigteone	0.927	0.005
		Vogelin – J	0.924	0.006
		Vogelin – B	0.922	0.006
		Vogelin – F	0.922	0.006
		Vogelin – A	0.914	0.008
		Vogelin – E	0.914	0.008
		Pterocarpan group - I	0.825	0.030
		Pterocarpan group - II	0.821	0.031
		1-Methoxyphaseolludin	0.792	0.038
2	HIF1A expression inhibitor	Vogelin – J	0.968	0.002
		Erysenegalensin – L	0.923	0.018
		Erysenegalensin – G	0.903	0.005
		Vogelin – I	0.871	0.007
		Pterocarpan group – II	0.842	0.009
		Erysenegalensin – F	0.674	0.023
3	CYP1A inhibitor	Isowigteone	0.953	0.002
		Vogelin – A	0.952	0.003
		Vogelin – B	0.934	0.003
		Vogelin – F	0.934	0.003
		Vogelin – G	0.890	0.004
		Vogelin – H	0.733	0.004
4	CYP1A1 inhibitor	Vogelin – B	0.962	0.001
		Vogelin – F	0.962	0.001
		Vogelin – A	0.957	0.001
		Isowigteone	0.946	0.001
5	Monophenol monooxygenase inhibitor	Isowigteone	0.977	0.001
		Vogelin – B	0.972	0.001
		Vogelin – F	0.972	0.001
		Vogelin – A	0.963	0.001
6	Aspulvinone dimethyl allyltransferase inhibitor	Pterocarpan group - II Pterocarpan group – I	0.848 0.753	0.020 0.047

7	Ubiquinol-cytochrome-c reductase inhibitor	Vogelin – B Vogelin – F Vogelin – H Erysenegalensin - F Erysenegalensin – M	0.898 0.898 0.784 0.761 0.716	0.005 0.005 0.038 0.046 0.063
8	MMP9 expression inhibitor	Isowigteone Vogelin – A Vogelin – B Vogelin – F Vogelin – G Erysenegalensin - F Erysenegalensin – G Erysenegalensin – L Vogelin – H Erysenegalensin – M	0.906 0.898 0.887 0.887 0.886 0.775 0.745 0.742 0.718 0.663	0.001 0.001 0.002 0.002 0.002 0.004 0.004 0.004 0.005 0.009
9	Apoptosis agonist	1-methoxyphaseolludin Erysenegalensin - F Pterocarpan group – I Vogelin – H	0.794 0.775 0.751 0.718	0.009 0.008 0.011 0.013

Table-1b: PASS prediction activity of flavonoids

S.No	Name of activity	Name of the flavonoids	PASS values 90%)	P_a/P_i (>65-
			P_a	P_i
10	Histidine kinase inhibitor	Isowigteone Vogelin – A Vogelin – B Vogelin – F Vogelin – G Erysenegalensin - F Erysenegalensin – G Vogelin – H Vogelin – I Erysenegalensin – M Erysenegalensin – L Vogelin – E	0.944 0.937 0.934 0.934 0.913 0.910 0.897 0.888 0.874 0.874 0.873 0.764	0.001 0.001 0.001 0.001 0.002 0.002 0.002 0.002 0.003 0.003 0.003 0.005
11	UGT1A10 substrate	Isowigteone Vogelin – B Vogelin – F Vogelin – A	0.953 0.952 0.951 0.924	0.002 0.002 0.002 0.002
12	TP53 expression inhibitor	Vogelin – J Vogelin – E Erysenegalensin – F	0.855 0.767 0.681	0.007 0.015 0.030
13	CF transmembrane conductance regulator agonist	Erysenegalensin - F Erysenegalensin – G Erysenegalensin – M Vogelin – I	0.786 0.744 0.698 0.654	0.002 0.003 0.003 0.002
14	Chemopreventive	Vogelin – I Erysenegalensin – L Vogelin – H Vogelin – E Erysenegalensin – G Erysenegalensin – M	0.813 0.789 0.788 0.774 0.708 0.682	0.004 0.004 0.004 0.004 0.006 0.007
15	Chalcone isomerase inhibitor	Vogelin – A Isowigteone Vogelin – B Vogelin – F	0.931 0.930 0.922 0.922	0.001 0.001 0.001 0.001

16	CDP – glycerol glycerophosphotransferase inhibitor	1-methoxyphaseolludin Vogelin – G Vogelin – E Erysenegalensin – G	0.892 0.889 0.792 0.726	0.011 0.012 0.032 0.047
17	UDP – glycuroxnosyl transferase substrate	Vogelin – H Vogelin – E	0.776 0.743	0.009 0.011
18	Lipid peroxidase inhibitor	Vogelin – G 1-methoxyphaseolludin Vogelin – H Erysenegalensin – L Vogelin – I	0.904 0.807 0.733 0.732 0.667	0.003 0.003 0.004 0.004 0.006

Table-1c: PASS prediction activity of flavonoids

S.No	Name of activity	Name of the flavonoids	PASS values P_a/P_i (>65-90%)	
			P_a	P_i
19	Aldehyde oxidase inhibitor	Vogelin – A Vogelin – B Vogelin – F Isowigteone Erysenegalensin – F Erysenegalensin – L Vogelin – I	0.913 0.895 0.895 0.894 0.857 0.707 0.704	0.004 0.004 0.004 0.004 0.006 0.017 0.017
20	Skin whitener	Vogelin – E 1-methoxyphaseolludin	0.797 0.795	0.001 0.001
21	CYP1A substrate	Vogelin – A Vogelin – G	0.891 0.890	0.004 0.004
22	CYP2E substrate	Erysenegalensin – L Vogelin – G Erysenegalensin – M	0.948 0.906 0.833	0.003 0.004 0.005
23	Anticarcinogenic	Erysenegalensin - L Erysenegalensin – M	0.770 0.663	0.006 0.010
24	AR expression inhibitor	Erysenegalensin - L Vogelin - I	0.708 0.660	0.005 0.007
25	Antineoplastic	1-methoxyphaseolludin Erysenegalensin – F Erysenegalensin – G Pterocarpan group – I Erysenegalensin –M Vogelin – I	0.851 0.848 0.808 0.756 0.732 0.662	0.018 0.007 0.007 0.004 0.021 0.033

III. MATERIAL AND METHODS:

Various constituents of Erythrina Varigata leave extracts reported were used for predicting bioactivity using PASS [15].Flavonoids are Pterocarpan group-I, Pterocarpan group-II, Isowigteone,1-methoxyphaseolludin,Vogelin-A,Vogelin-B,Vogelin-E,Vogelin-F,Vogelin-G,Vogelin-H,Vogelin-I,Vogelin-J,Erysenegalensin-G,Erysenegalensin-L,Erysenegalensin-M and Erysenegalensin-F.

IV. RESULT AND DISCUSSION

Prediction of bioactivity result for Erythrina Varigata leaf Constituents were predicted in **Table-1a, 1b and 1c.**

All the compounds (1-16) isolated from Erythrina Varigata leaf extract were found to exhibit under PASS prediction activities [15]. Membrane integrity agonist, HIF1A expression inhibitor, CYP1A inhibitor, CYP1A1 inhibitor, Monophenol monooxygenase inhibitor, Aspulvinone dimethyl allyltransferase inhibitor, Ubiquinol-cytochrome-c reductase inhibitor, MMP9 expression inhibitor, Apoptosis agonist, Histidine kinase inhibitor, UGT1A10 substrate, TP53 expression inhibitor, CF transmembrane conductance regulator agonist, Chemopreventive, Chalcone isomerase inhibitor, CDP – glycerol glycerophosphotransferase inhibitor, UDP – glycuroxnosyl transferase substrate, Lipid peroxidase inhibitor, Aldehyde oxidase inhibitor, Skin whitener, CYP1A substrate, CYP2E substrate, Anticarcinogenic, AR expression inhibitor, Antineoplastic were found to above >65-90% as given in **Table- 1a, 1b and 1c.**

Membrane integrity agonist

PASS prediction of the membrane integrity agonist activity of Isowigteone (0.927), Vogelin-J (0.924), Vogelin-B (0.922), Vogelin-F (0.922), Vogelin-A (0.914) and Vogelin-E (0.914) were found to greater than 90% of Pa activities. Flavonoids

are Pterocarpan group-I (0.825), Pterocarpan group-II (0.821) and 1-methoxyphaseolludin (0.792) were found to less than 90% of activities.

HIF1A expression inhibitor

Activities for Vogelin – J, Erysenegalensin – L, Erysenegalensin – G, Vogelin – I, Erysenegalensin – F and Pterocarpan group – II were found to greater than 90% of PASS prediction activity of HIF1A expression inhibitor.

CYP1A inhibitor

Prediction activity of flavonoids are Isowigteone, Vogelin – A, Vogelin – B, Vogelin – F, Vogelin – G and Vogelin – H were shown in 95.3%, 95.2%, 93.4%, 93.4%, 89% and 73.3% of CYP1A inhibitor activities.

CYP1A1 inhibitor

PASS predictions of flavonoids are Vogelin – B, Vogelin – F, Vogelin – A and Isowigteone were predicted to greater than 90% of CYP1A1 inhibitor activities.

Monophenol monooxygenase inhibitor

Activity in the Monophenol monooxygenase inhibitor of Isowigteone, Vogelin – B, Vogelin – F and Vogelin – A were shown in 97.7%, 97.2%, 97.2% and 96.3 of prediction activities.

Aspulvinone dimethyl allyltransferase inhibitor

The aspulvinone dimethyl allyltransferase inhibitor for Pterocarpan group – II and Pterocarpan group – I were observed to have less than 90% of Pa value of activities.

Ubiquinol-cytochrome-c reductase inhibitor

Vogelin – B, Vogelin – F, Vogelin – H, Erysenegalensin – L and Erysenegalensin –M were found to greater than 70% for the ubiquinol- cytochrome-c reductase inhibitor.

MMP9 expression inhibitor

PASS prediction activity in the MMP9 expression inhibitor of Isowigteone were observed to have high Pa value than other flavonoids are Vogelin – A, Vogelin – B, Vogelin – F, Vogelin – G, Erysenegalensin – F, Erysenegalensin – G, Erysenegalensin – L, Erysenegalensin – M and Vogelin – H were found to less than (<90%) of activities.

Apoptosis agonist

The apoptosis agonist for 1-methoxyphaseolludin, Erysenegalensin – F, Pterocarpan group – I and Vogelin – H were predicted in 79.4, 77.5, 75.1, and 71.6% of activities in **Table -1a.**

Histidine Kinase inhibitor

Activity for Isowigteone, Vogelin – A, Vogelin –B, Vogelin – F, Vogelin – G, Erysenegalensin – F, Erysenegalensin – G, Vogelin – H, Vogelin – I, Erysenegalensin – M, Erysenegalensin – L, Vogelin – E were shown in 94.4, 93.7, 93.4, 93.4, 91.3, 91.0, 89.7, 88.8, 87.4,87.4, 87.3 and 76.4% for the histidine kinase inhibitor.

UGT1A10 substrate

The UGT1A10 substrate for Isowigteone (0.953), Vogelin – B (0.952), Vogelin – F (0.951) and Vogelin – A (0.924) were found to greater than 90% of prediction activities.

TP53 expression inhibitor

Prediction activity of the TP53 expression inhibitor of Vogelin – J, Vogelin – E and Erysenegalensin – F were observed to have some small Pa value of 0.855, 0.767 & 0.681 activities.

CF transmembrane conductance regulator agonist

Erysenegalensin – F (0.786), Erysenegalensin – G (0.744), Erysenegalensin – M (0.698) and Vogelin – I (0.654) were found to be range of higher than (>65%) and lower than (<80%) of the prediction activity for CF transmembrane conductance regulator agonist.

Chemopreventive

PASS prediction activity of the chemopreventive of Vogelin – I, Erysenegalensin – L, Vogelin – H, Vogelin – E, Erysenegalensin – G and Erysenegalensin – M were shown in **Table 1b**.

Chalcone isomerase inhibitor

Chalcone isomerase inhibitor for Vogelin – A (93.3%), Isowigteone (93%), Vogelin – B (92.2%) and Vogelin – F (92.2%) were found to greater than (>90%) of PASS prediction activities.

CDP – glycerol glycerophosphotransferase inhibitor

Activity for 1- methoxyphaseolludin, Vogelin – G, Vogelin – E and Erysenegalensin – G were shown in Pa value of **Table-1b**.

UDP – glycuroxnosyl transferase substrate

The UDP – glycuroxnosyl transferase substrate Vogelin – H and Vogelin – E were predicted in the Pa value 77.6 and 74.3% of activities.

Lipid peroxidase inhibitor

Vogelin – G, 1- methoxyphaseolludin, Vogelin – H, Erysenegalensin – L and Vogelin – I were found to be the range of greater than 65% for the lipid peroxidase inhibitor.

Aldehyde oxidase inhibitor

Activity of the aldehyde oxidase inhibitor of Vogelin – A (0.913), Vogelin – B (0.895), Vogelin – F (0.895), Isowigteone (0.894), Erysenegalensin – F (0.857), Erysenegalensin – L (0.707) and Vogelin – I (0.704) were calculated to have greater than 70% of prediction activities.

Skin whitener

Skin whitener for Vogelin – E (0.797) and 1- methoxyphaseolludin (0.795) were observed to have almost same Pa value 79% of PASS prediction activities.

CYP1A substrate

Vogelin – A and Vogelin – G were found to have same activity of Pa value 0.891 & 0.890 for the CYP1A substrate.

CYP2E substrate

The CYP2E substrate for Erysenegalensin – L (0.948), Vogelin – G (0.906) and Erysenegalensin – M (0.833) were predicted to greater than 80% of activities.

Anticarcinogenic

PASS prediction activity of the anticarcinogenic of Erysenegalensin – L and Erysenegalensin – M were shown in **Table-1c**.

AR expression inhibitor

AR expression inhibitor for Erysenegalensin –L (0.708) and Vogelin – I (0.667) were found to greater than 65% of activities.

Antineoplastic

Activity for 1- methoxyphaseolludin, Erysenegalensin –F, Erysenegalensin –G, Pterocarpan group – I, Erysenegalensin – M and Vogelin – I was shown in **Table-1c.**

CONCLUSION

The various flavonoids with pharmacological activities isolated from Erythrina Varigata leave extract were predicted using the PASS online software. All the sixteen flavonoids were calculated from Erythrina varigata leave, Vogelin – A and Isowigteone were found to more activity of Membrane integrity agonist (91.4, 92.6%), CYP1A inhibitor (95.2, 95.3%), CYP1A1 inhibitor (95.7%), Monophenol monooxygenase inhibitor (96.3, 97.7%), MMP9 expression inhibitor (89.8, 90.6%), Histidine kinase inhibitor (93.7, 94.4%), UGT1A10 substrate (92.4, 95.3%), Chalcone isomerase inhibitor (93.1, 93.0%), Aldehyde oxidase inhibitor (91.3, 89.4%), CYP1A substrate (89.1%) results were showed by PASS prediction activities.

REFERENCES

[1] Viji M, Murugesan S. Phytochemical analysis and antibacterial activity of medicinal plant *Cardiospermum halicacabum* Linn. Pytopharmacol. 2010; 2:68-77.
[2] Rasdi N.H.M, Samah O.A, Sule A, Ahmed Q.U. Antimicrobial studies of *Cosmos caudatus* Kunth (Compositae). J Med Plant Res., 2010; 4: 669 – 673.
[3] Chopra, I., Hodgson, J., Metcalf, B., Poste, G., New approaches to the control of infectious caused by antibiotic resistant bacteria. An industry prespective. J. Am. Med.Assoc., 1996. 275: 401 – 403.
[4] Baquero, F., Gram – positive resistance: Challenges for the development of new antibiotics. J. Antimicrob. Chemother. 1997. 39: 1-6.
[5] Kamatou, G.P.P., Van Vuuren, S.F., Van Heerden, F.R., Seaman, T., Viljoen, A.M.,Antibacterial and anti mycobacterial activities of South African Salvia species and isolated compounds from S.Chamelaeagnea. S. Afr. J. Bot., 2007; 73: 552-557.
[6] Srinivasan, D., Nathan, S., Suresh, T., Perumalsamy, O., Antimicrobial activity of certain Indian medicinal plants used in folkloric medicine. Journal of Ethnopharmacology., 2001. 74: 217–220.
[7] Kumarasamy, Y., Cox, P., Jaspars, M., Nahar, L., Sarker, S., Screening seeds of Scottish plants for antibacterial activity. Journal of Ethnopharmacology., 2002. 83: 73–77.
[8] Ali, N.A.A., Julich, W.D., Kusnick, C., Lindequist, U., Antimicrobial and phytochemical studies on 45 Indian medicinal plants against multi-drug resistant human pathogens. Journal of Ethnopharmacology., 2001. 74: 113–123.
[9] Masika, P.J., Afolayan, A.J., Antimicrobial activity of some plants used for the treatment of livestock disease in the Eastern Cape, South Africa. Journal of Ethnopharmacology., 2002. 83: 129–134.
[10] Hamill, F.A., Apio, S., Mubiru, N.K., Bukenya-Ziraba, R., Mosango, M., Maganyi, O.W.,Soejarto, D.D., Traditional herbal drugs of Southern Uganda, II: literature analysis and antimicrobial assays. Journal of Ethnopharmacology., 2003; 84: 57–78.
[11] Shereen Ledman, M.S., Nutrition Expert, Flavonoids Nutrition Glossary., updated April 28, 2014.

[12] Poroikov, V., Akimov, D., Shabelnikova, E., and Filimonov, D., *SAR and QSAR in Environmental Research*, 2001; (4), 327-344.
[13] Oruc, E., Rollas, S., Kandemirili, F., Shvets, N., and Dimoglo, A.S., *J.Med.Chem*, 2004; 47, 6760-6767.
[14] Http:// www.ibmc.msk.ru/PASS.
[15] Behrangi N., Hashemi M., Dourtar Y., and Borna H.Camptothecins and their Novel Properties Evaluated by using Pass Method. Advances in Environmental Biology, 2011; 5(9): 2551-2556.

