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Pharmacological activities assessment using pass for fewer alkaloids of Erythrina varegate

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Abstract
Pharmacological activities of the ten alkaloids present in Erythrina variegate were assessed using PASS software. PASS prediction result showed that these alkaloids were found to exhibit various pharmacological activities like 5-hydroxytypaminestimulant(92.9%), Chlordecone release stimulant (89.1%),aspulvinone dimethyl allyl stimulant (89.1%), fibrinolytic (86.1%),MAP kinase stimulant (84.3%),antidyskinetic (84.0%),Taurine dehydrogenase inhibitor (83.6%) as their highest scores.

Keywords: PASS, Erythrina variegate, alkaloids, antidyskinetic.

Introduction

The Erythrina variegate belongs to the Fabaceae family [1] and the alkaloids present in it [2] finds its importance as traditional medicine to cure various diseases like nervine sedative, ophthalmic, asthma, epilepsy, and antiseptic. Its leaves have a cathartic, diuretic, antiseptic, anti-inflammatory and analgesic activity, convulsion, fever, inflammation, bacterial infection, insomnia, helminthiasis, cough, cuts and wounds [3-6]. E. variegate shows several other characteristic pharmacological effects like neuromuscular blocking, smooth muscle relaxant, CNS depressant, analgesic and hydrocholerectic action. Knowing the various pharmacological activities of the alkaloids present in Erythrina variegate leaves and in continuation of our work in determining the binding energies to predict the stability of alkaloids by computational chemistry, our present work is focussed on the assessment of pharmacological activities using PASS software. [7]

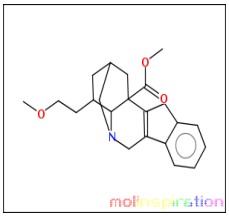
In PASS (Prediction of Activity Spectra for Substance) the biological activity spectrum for a alkaloid was asserted on the basis of its structural formula [8-10]. The values of Pa (probability to be active) estimates the chance that the studied compound is belonging to the sub-class of active compounds resembles the structures of molecules and Pi (probability to be inactive) estimates the chance that the studied compound is belonging to the sub-class of inactive compounds resembles the structures of molecules.

Materials and methods

Ten alkaloids present in Erythrina variegate were selected and their structures were drawn using molinspiration software for the

assessment of pharmacological activities using PASS.

The structures of ten alkaloids were given in fig I – X as follows: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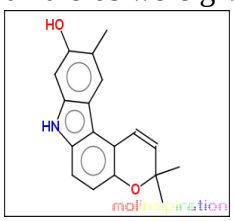
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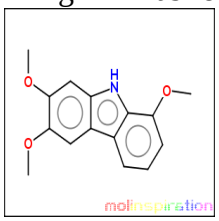
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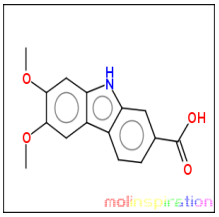
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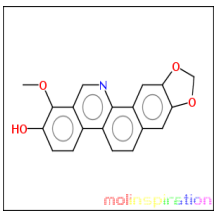
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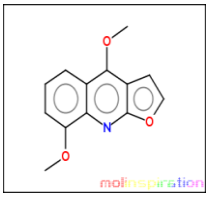
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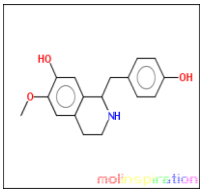
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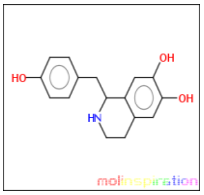
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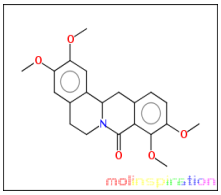
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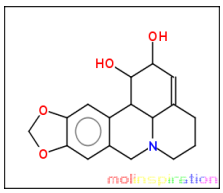
X

Table 1a: PASS prediction activity.

Sr. No.	Name of the activity	Alkaloids	PASS values	
			Pa	Pi
1	5-hydroxy tryptamine release stimulant	III	0.929	0.004
		IX	0.918	0.017
		VIII	0.835	0.011
		VII	0.775	0.004
2	Antidyskinetic	IX	0.840	0.028
		VII	0.800	0.005
		VIII	0.799	0.005
		X	0.741	0.004
		II	0.646	0.011
3	Anti neoplastic	V	0.730	0.021
		X	0.718	0.005
		II	0.661	0.033
4	Nicotinic alpha 6 beta 3 beta4 alpha5 receptor antagonist	VII	0.835	0.006
		VIII	0.707	0.033
5	MAP kinase stimulant	IX	0.843	0.003
		V	0.787	0.003
		VII	0.730	0.005
		X	0.723	0.005
		VIII	0.703	0.005
6	Histamine release stimulant	VII	0.746	0.004
		VIII	0.696	0.004
7	Fibrinolytic	VII	0.867	0.004
		VIII	0.843	0.004
8	JAK2 expression inhibitor	III	0.763	0.011
		V	0.709	0.016
		VII	0.692	0.018
		VI	0.527	0.047

9	Cytochrome P450 stimulant	III	0.786	0.004
		II	0.659	0.009
10	Chlordecone reductase inhibitor	IV	0.891	0.006
		III	0.808	0.019

Table 1b: PASS prediction activity.

Sr. No.	Name of the activity	Alkaloids	PASS values	
			Pa	Pi
11	Caspace-8-stimulant	V	0.796	0.006
		VI	0.482	0.021
12	Ubiquinol-cytochrome-c-reductase inhibitor	III	0.793	0.035
		VI	0.751	0.050
13	Taurine dehydrogenase inhibitor	IV	0.836	0.008
		VI	0.567	0.066
14	Ovulation inhibitor	V	0.608	0.016
		X	0.601	0.017
15	Antiprotozoal	VI	0.718	0.008
		X	0.545	0.008
16	Membrane integrity agonist	VIII	0.717	0.052
		X	0.680	0.058
17	Glutamate-5-semialdehyde dehydrogenase inhibitor	VIII	0.746	0.022
		VII	0.644	0.034
18	Gluconate -2-dehxydrogenase inhibitor	III	0.818	0.012
		IX	0.731	0.040
		VII	0.676	0.071
19	Neuro transmitter uptake inhibitor	X	0.723	0.009
		V	0.635	0.022
20	Aspulvinone dimethyl allyl transferase inhibition	III	0.891	0.010
		V	0.788	0.037
		VI	0.782	0.039

Results and discussion

Pharmacological activity assessment results for Erythrina variegate alkaloids were listed in **Table-1a and 1b**.

(a) 5-hydroxy tryptamine release stimulant

The role of 5-hydroxy tryptamine release stimulant is to stimulate respiration in dogs Alkaloid III (0.929), IX (0.918), VIII (0.835) and VII (0.775) were found to exhibit 5-hydroxy tryptamine release stimulant activity.

(b) Anti dyskinetic

Anti dyskinetic activity plays a vital role as deep brain stimulant. Alkaloid IX (84.0%), VII (80.0%), VIII (79.9%) ,X (74.1%) and II (64.6%) showed antidyskinetic activity.

(c) Nicotinic alpha 6 beta 3 beta4 alpha5 receptor antagonist

Nicotinic alpha 6 beta 3 beta4 alpha5 receptor antagonist was a type of nicotinic acetylcholine receptor, located in the brain, associated with growth hormone secretion. Alkaloid VII (83.5%) and VIII (70.7%) showed this activity.

(d) MAP kinase stimulant

Mitogen Activated Protein (MAP) kinase stimulant plays an important role in cell growth. Alkaloid IX (84.3%), V (78.7%), VII (73.0%), VIII (70.3%), and X (72.3%) showed MAP kinase activity.

(e) Histamine release stimulant activity

Histamine is the gastric mucosa acts as a local chemical mediator for other gastric

stimulants. For alkaloid VII the activity was 74.6% and VIII it was 69.6%.

(f) Fibrinolytic activity

Alkaloid VII showed 86.7% and VIII showed 84.3% fibrinolytic activity.

(g) Chlordecone reductase inhibitor

Chlordecone reductase inhibitor activity of alkaloid IV was 89.1% and III was 80.8%.

(h) Taurine dehydrogenase inhibitor Activity

The Taurine dehydrogenase inhibitor counteracts oxidative stress and nerve growth factor deficit in diabetic neuropathy. The alkaloid IV showed 83.6% activity.

(i) Gluconate -2-dehxydrogenase inhibitor Activity

The Gluconate -2-dehxydrogenase inhibitor activity of the alkaloid III, VI and IX were found to be 81.8%, 67.6 % and 73.1% respectively.

(j) Aspulvinone dimethyl allyl transferase inhibitor

Aspulvinone dimethyl allyl transferase was a prenylation enzyme for the biosynthesis of aspulvinone pigments as they are potent anti-influenza H_1N_1 virus. Alkaloid III (0.891) was found to posse's 90% inhibitor activity.

Conclusion

The pharmacological activities of ten alkaloids isolated from Erythrina variegate extract were asserted using PASS software and found to exhibit the twenty different pharmacological activities ranges from 71.7% to 92.9% .The highest scores were observed as 5-hydroxytryptamine stimulant(92.9%), Chlordecone release stimulant(89.1%), aspulvinone dimethyl allyl stimulant (89.1%), Fibrinolytic (86.7%),MAP kinase stimulant (84.3%), Antidyskinetic (84.0%), Taurine dehydrogenase inhibitor(83.6%), Nicotinic alpha 6 beta 3 beta 4 alpha 5 receptor antagonist (83.5%), gluconate -2-dehydrogenase inhibitor (81.8%). Among the ten alkaloids, alkaloid VIII was found to exhibit more pharmacological activities and hence it may find as a pharmacologically active drug among other alkaloids.

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