



Predicting The Potential of Convolvulus Pluricaulis Against Cognitive Dysfunction With The Help of Prediction of Activities Spectra of Substances Software

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ABSTRACT

Objective: Cognitive dysfunction appertains to a loss in verbal, non-verbal learning, attention, working and short-term memory, motor functioning, problem-solving, and processing speed. The major objective of this study is to find out phytoconstituents obtained from Convolvulus Pluricaulis with the help of PASS software, which can be used in the treatment of cognitive dysfunction.

Methods: PASS is important software used in this study to find out biological activity spectra of phytoconstituents of Convolvulus Pluricaulis in the amelioration of cognitive dysfunction. The predicted biological activity was also compared with marketed compounds like Rivastigmine, donepezil, memantine, and curcumin.

Results: From the study, it was found that CP has great potential in the treatment of cognitive dysfunction. Many phytoconstituents of CP have free radical scavenging, antioxidant, and dementia treatment activity.

Conclusion: In this research work, information was compiled with the help of PASS software of phytoconstituents of Convolvulus Pluricaulis for its potential against cognitive dysfunction. Further research is required to explore the potential of CP phytoconstituents in the treatment of cognitive dysfunction..

1. Introduction

Cognitive dysfunction appertains to a loss in verbal, non-verbal learning, attention, working and short-term memory, motor functioning, problem-solving, and processing speed (Zhao et al., 2014). Cognitive dysfunction is commonly called as dementia. Globally, approximately forty million geriatric people are living with cognitive dysfunction. India is not far behind in numbers of people suffering from dementia, approximately 3.7 million people in India have cognitive dysfunction and the pervasiveness is anticipated to surge doubled by 2030 and tripled by 2050 (Mehla et al., 2020). Cognitive dysfunction is linked with neurodegenerative diseases like epilepsy, schizophrenia, Alzheimer's disease (AD), Huntington's disease, and Parkinson's disease. Several herbal drugs are used to improve cognitive functions, Convolvulus Pluricaulis is one of them, it is known to improve memory. Several flavonoids, coumarins, and alkaloids are extracted from this herb, these active chemicals are responsible for pharmacological activities displayed by this medicinal herb.

PASS (Prediction of activity spectra for substances) web tool, which prognosticate more than 3678 pharmacological

outcomes, mechanisms, and various toxicities of a molecule including teratogenicity, mutagenicity, embryotoxicity, and carcinogenicity. This software predicts Pa: Pi (Probable activity: Probable inactivity) based on the structural formula of a substance. If Probable activity is greater than 0.7 for any activity, the chance of substance activity in the pharmacological examination is high. If Probable activity; Pa is greater than 0.5 but less than 0.7 ($0.5 < Pa < 0.7$) then the probability of that action in the pharmacological experiment is likely less. If $Pa < 0.5$, then the substance unlikely to exhibit any biological activity in the pharmacological experiment (Lagunin et al., 2000), (Parasuraman, 2011).

2. Methods

To evaluate activity using PASS software first, we select certain phytoconstituents present in Convolvulus Pluricaulis and which are reported to have pharmacological activities in the in vitro and in vivo experiments conducted for CP. PASS software will elucidate the pharmacological activity spectra using 2D structures of the molecules. The 2D Structures used are obtained from PubChem and are directly copied

into PASS software to predict the biological activity spectra of the molecule.

3. Results

The selected standard compounds and phytochemicals were predicted using PASS software for ten activities in cognitive dysfunction caused by neurodegenerative disorders. These activities are as follows:

1. Free radical scavengers
2. Dopamine release stimulant

3. Nootropic activity
4. COMT inhibitor
5. MAO inhibitor
6. Dementia treatment
7. Anti-amyloidogenic activity
8. Antiparkinsonian
9. Antiparkinsonian, tremor relieving activity
10. Anti-oxidant activity

Predicted Pa (Probable activity) predicted by PASS is represented in table 1 and also compared with standard drugs like Donepezil, Rivastigmine, Memantine, and Curcumin.

Table 1: Pa (Probable activity) predicted by PASS software.

Name of compound	Pa predicted by PASS software										
	Reported activity	Free radical scavenging activity	Dopamine release stimulant	Nootropic activity	Anti-parkinsonian	Catechol O methyl-transferase inhibitor	Monoamine oxidase inhibitor	Dementia treatment	Antia-amyloidogenic activity	Anti-parkinsonian, tremor relieving activity	Anti-oxidant
Curcumin	Cognition enhancer, ameliorates β -amyloid formation (Voulgaropoulou et al., 2019), (Mehla et al., 2020)	0.766	0.433	0.553	NP	0.121	0.118	0.352	NP	NP	0.61
Donepezil	Cognition enhancer, free radical scavenger ((PDF) Donepezil Improves Cognition and Global Function in Alzheimer Disease: A 15-Week, Double-Blind, Placebo-Controlled Study. Donepezil Study Group, n.d.), (Umukoro et al., 2014)	NP	0.165	0.553	0.228	NP	NP	0.301	NP	0.19	NP
Rivastigmine	Cognition enhancer (Annicchiarico et al., 2007)	NP	0.226	0.694	NP	0.051	0.365	NP	NP	0.266	NP
Memantine	Improve memory impairment (Ramaswamy et al., 2015)	NP	0.515	NP	0.807	NP	NP	0.416	NP	NP	NP

Subhirsine	Memory enhancement (Shelke & Jitendra Joshi, 2020)	0.213	0.314	NP	0.23	NP	NP	0.267	0.44	0.321	0.15
Convolvine	Nootropic activity (<i>Sci-Hub Neuro-and Psychopharmacological Investigation of the Alkaloids Convolvine and Atropine. Chemistry of Natural Compounds</i> , 34(1), 56–58 10.1007/Bf02249687, n.d.)	0.275	0.366	0.434	0.261	NP	NP	0.308	0.345	0.302	0.165
Confoline	Inhibition of ACHE level and β -amyloid plaque formation (Balkrishna et al., 2020)	0.188	0.262	0.476	NP	NP	NP	0.247	0.263	0.272	0.135
Convalidine	Inhibition of ACHE level and β -amyloid plaque formation (Shelke & Jitendra Joshi, 2020)	0.406	0.419	0.39	0.263	0.072	NP	0.284	0.326	0.296	0.244
Convolamine	Cognition enhancer (Balkrishna et al., 2020)	0.237	0.311	0.48	0.344	NP	NP	0.377	0.435	0.525	0.16
Convoline	Inhibition of ACHE level and β -amyloid plaque formation (Shelke & Jitendra Joshi, 2020)	0.376	0.262	NP	NP	NP	NP	0.248	0.29	0.185	0.184
Kaempferol	Decrease dopaminergic neuron loss, increases SOD and GPx activity (Ren et al., 2019)	0.771	0.217	0.348	NP	0.072	0.538	0.374	NP	NP	0.856
Scopoletin	Cognition enhancement property (Ariane Hornick et al., 2008), (A. Hornick et al., 2011)	0.742	0.351	0.345	NP	0.078	0.488	0.354	NP	0.282	0.54
Cinnamic acid	Decrease dopaminergic neuron loss (Bae et al., 2018)	0.497	0.293	NP	NP	0.064	0.114	0.383	NP	0.224	0.489

Decanoic acid	Cognition enhancer, seizure controls by directly inhibiting AMPA receptor (Chang et al., 2016), (Wang & Mitchell, 2016)	0.315	0.36	0.525	NP	0.061	NP	0.405	0.249	0.345	0.222
Quercetin	Anti-oxidant, inhibit β -amyloid protein, cognition enhancer (Angélica Maria et al., 2015), (Angélica Maria et al., 2015)	0.811	0.215	0.341	NP	0.107	0.436	0.327	NP	NP	NP
Ayapanin	Nootropic activity	0.602	0.331	0.402	NP	NP	0.583	0.423	0.218	0.296	0.437
Squalene	Anti-oxidant and anti-depressant (Sasaki et al., 2019)	0.456	0.346	0.407	NP	NP	0.111	0.613	NP	0.192	0.657
Delphinidin	Anti-oxidant, ameliorates β -amyloid formation (Masheta & Al-Azzawi, 2018), (Kim et al., 2009)	NP	0.165	0.553	0.228	NP	NP	0.301	NP	0.19	NP
Phthalic acid	Neuroprotective action (S & Shivanandappa, 2018)	0.303	0.362	0.385	NP	0.048	NP	0.48	0.425	0.37	0.161
2-Pentanol	Suppress formation and release of β -amyloid peptide (Wu et al., 2014)	0.219	0.335	0.479	NP	NP	NP	0.51	0.317	0.399	0.238
Pentanoic acid	Decrease dopaminergic neuron loss (Jayaraj et al., n.d.)	0.315	0.36	0.525	NP	0.061	NP	0.405	0.249	0.345	0.222
Vitamin-E	Anti-oxidant, cognition enhancer, reduced risk of developing AD (Fata et al., 2014)	0.607	NP	NP	NP	NP	NP	NP	NP	NP	0.967
Ascorbic acid	cognition enhancer, anti-oxidant (Bowman, 2012), (Travica et al., 2017)	0.564	0.222	0.571	NP	NP	NP	0.315	NP	0.138	0.928

Discussion

We have compared our results with earlier studies, CP is an important medicinal herb, phytoconstituents present in this plant has shown potential to treat cognitive dysfunction

linked with neurodegenerative diseases like AD, Parkinson's disease, epilepsy, Huntington's disease, etc. PASS software provides information about a particular compound, which can be valuable in a certain disease. Four standard drugs were taken (Curcumin, Donepezil, Rivastigmine, Memantine) to

compare with the phytoconstituents. All compounds were tested for ten activities (fig.1). We found that quercetin has the highest free radical scavenging activity (fig. 2). The phytoconstituents which show free radical scavenging activity follows the pattern quercetin > kaempferol >

curcumin > scopoletin > vitamin-E > ayapanin > ascorbic acid > cinnamic acid > squalene > convolidine > convolvine > pentanoic acid = decanoic acid > phthalic acid > convolvine > convolamine > 2-pentanol > subhirsine > confoline.

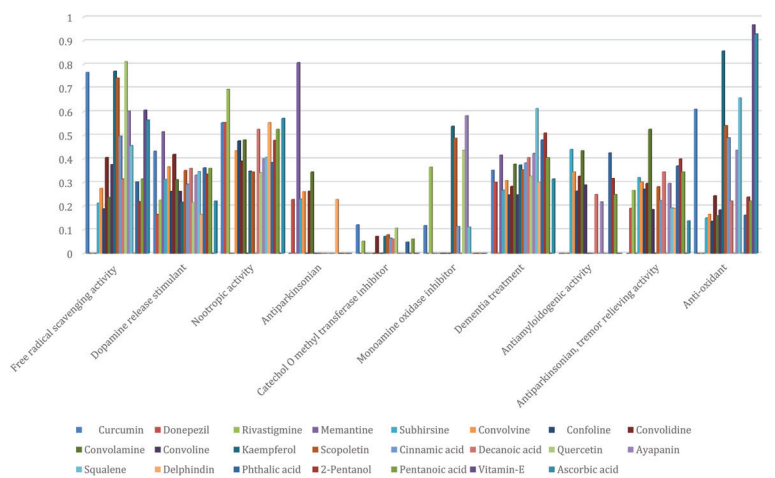


Figure 1: All activities of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

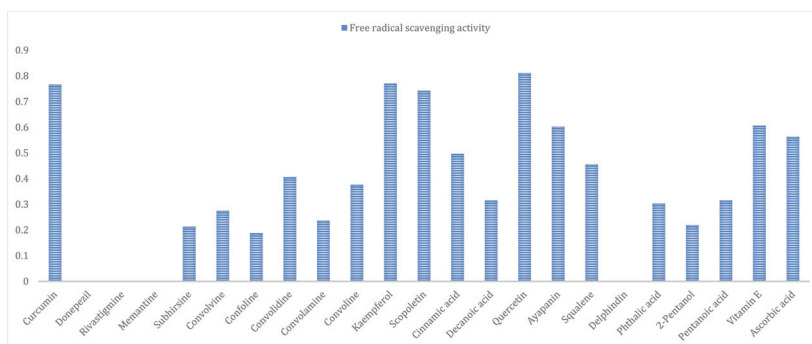


Figure 2: Free radical scavenging activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

Memantine was found to have the highest DA release stimulant activity when compared with other compounds (fig. 3). Convolidine was found to have the highest value among the phytochemicals of CP. Other compounds having DA release activity are as follow: Memantine > curcumin

> convolidine > convolvine > phthalic acid > pentanoic acid = decanoic acid > scopoletin > squalene > 2-pentanol > ayapanin > subhirsine > convolamine > cinnamic acid > convolvine = confoline > rivastigmine > ascorbic acid > kaempferol > quercetin > donepezil = delphinidin.

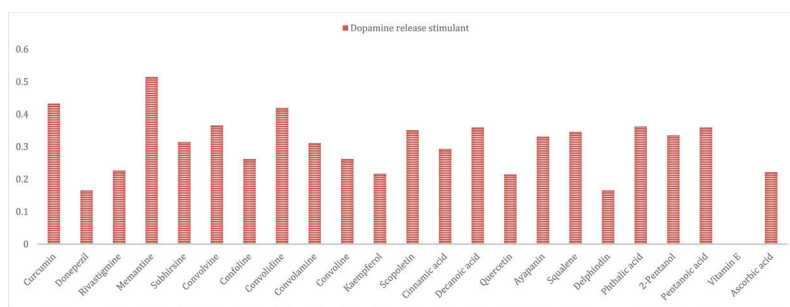


Figure 3: Dopamine release stimulant activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

Nootropic activity shown in fig. 4 follow the order: Rivastigmine > ascorbic acid > curcumin = donepezil = delphindin > decanoic acid = pentanoic acid > convolamine

> 2-pentanol > confoline > convolvine > squalene > ayapanin > convolidine > phthalic acid > kaempferol > scopoletin > quercetin.

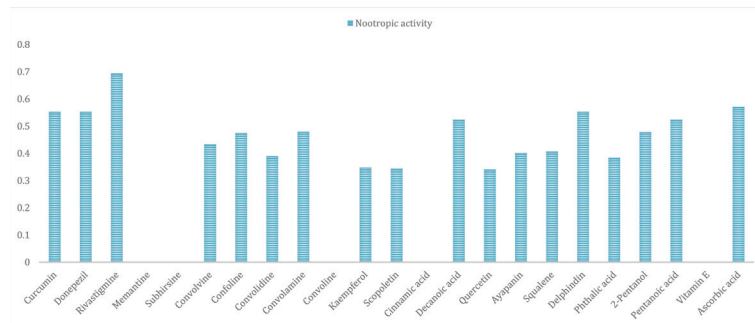


Figure 4: Nootropic activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

Only 5 phytoconstituents of CP has shown antiparkinsonian activity (fig. 5) which is as follow: Memantine >

convolamine > convolidine > convolvine > subhirsine > donepezil=delphindin.

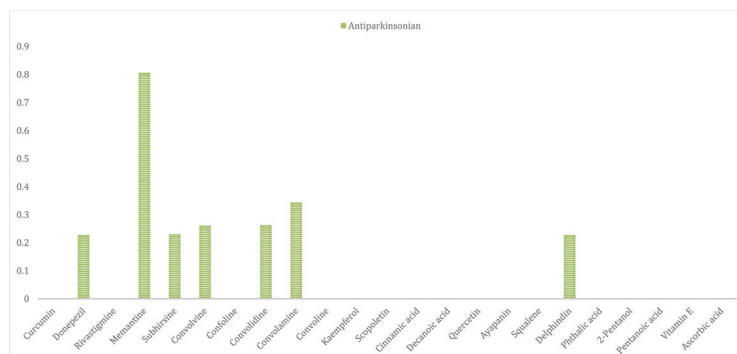


Figure 5: Antiparkinsonian activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

Again in the case of antiparkinsonian, tremor relieving activity convolamine has the highest value (fig. 6) and according to the value list is like: Convolamine > 2-pentanol > phthalic acid > pentanoic acid = decanoic acid > subhirsine

> convolvine > convolidine = ayapanin > scopoletin > confoline > rivastigmine > cinnamic acid > squalene > delphindin = donepezil > convoline > ascorbic acid.

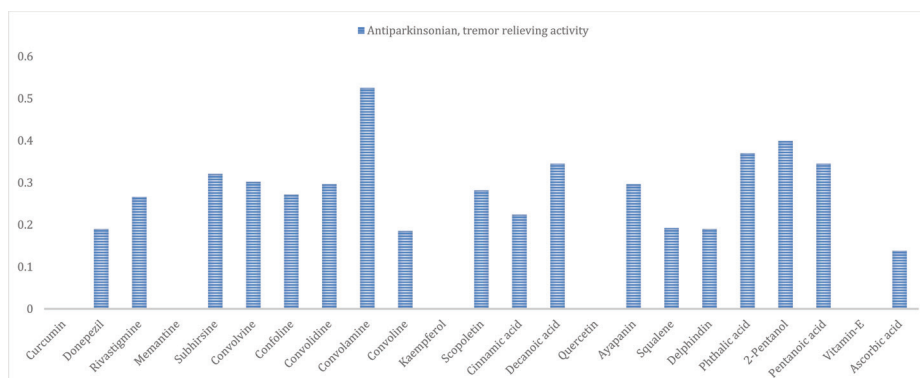


Figure 6: Antiparkinsonian, tremor relieving activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

COMT inhibitor activity is found to be very low (fig. 7) and follows the order: Curcumin > quercetin > scopoletin >

kaempferol = convolidine > cinnamic acid > pentanoic acid = decanoic acid > rivastigmine > phthalic acid.

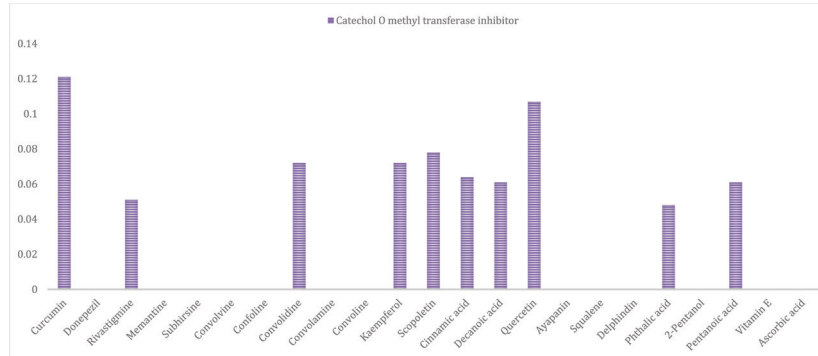


Figure 7: COMT inhibitor activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

In MAO inhibiting activity, Ayapanin has the highest value than other phytochemicals: Ayapanin > kaempferol > scopoletin > quercetin > rivastigmine > curcumin > cinnamic acid > squalene (fig. 8). In dementia treatment activity of squalene is highest among all phytoconstituents including 4 standard drugs (fig.9). Squalene > 2-pentanol >

phthalic acid > ayapanin > pentanoic acid = decanoic acid > cinnamic acid > convolamine > kaempferol > scopoletin > curcumin > quercetin > ascorbic acid > convolvine > donepezil = delphinidin > convolidine > subhirsine > convoline > confoline.

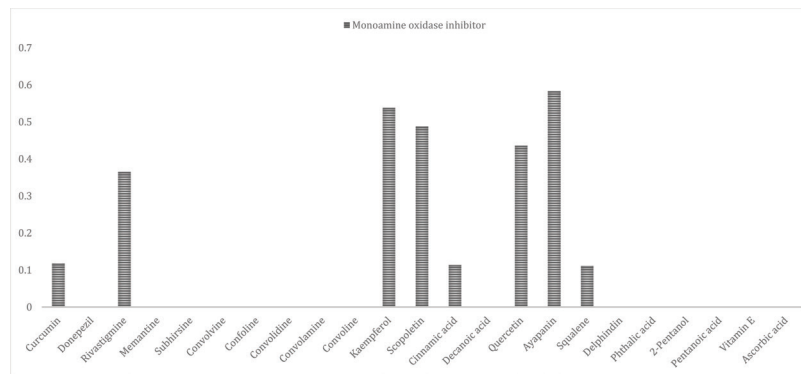


Figure 8: MAO inhibitor activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

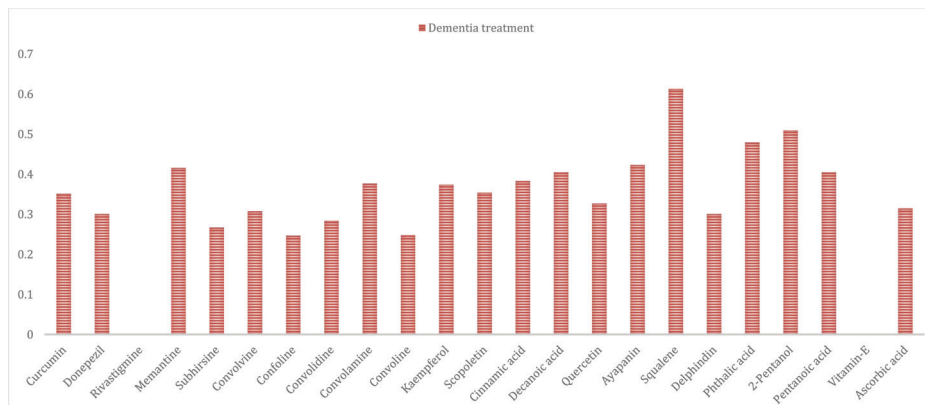


Figure 9: Dementia treatment activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

In case of anti-amyloidogenic activity eleven phytoconstituents were found to have anti-amyloidogenic activity shown in fig. 10. The phytoconstituents which has shown this activity

follows the pattern: Subhirsine > convolamine > phthalic acid > convolvine > convolidine > 2-pentanol > convoline > confoline > pentanoic acid = decanoic acid > ayapanin.

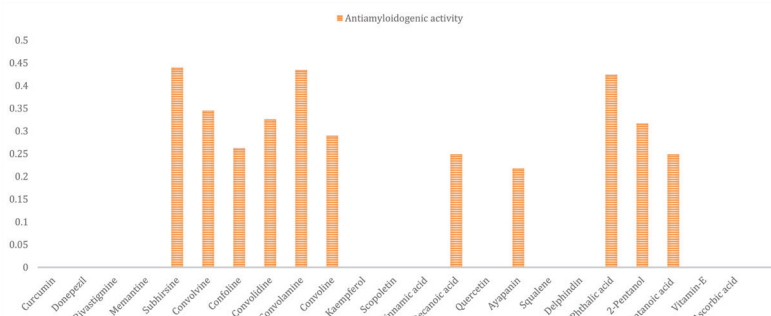


Figure 10: Anti-amyloidogenic activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

Out of 4 standard drugs, only curcumin has shown anti-oxidant activity, and in the phytochemicals of CP, Vitamin-E has the highest activity (fig. 11). The order of antioxidant activity for all compounds: Vitamin-E > ascorbic acid >

kaempferol > squalene > curcumin > scopoletin > cinnamic acid > ayapanin > 2-pentanol > convolidine > pentanoic acid = decanoic acid > convoline > convolvine > phthalic acid > convolamine > subhirsine > confoline.

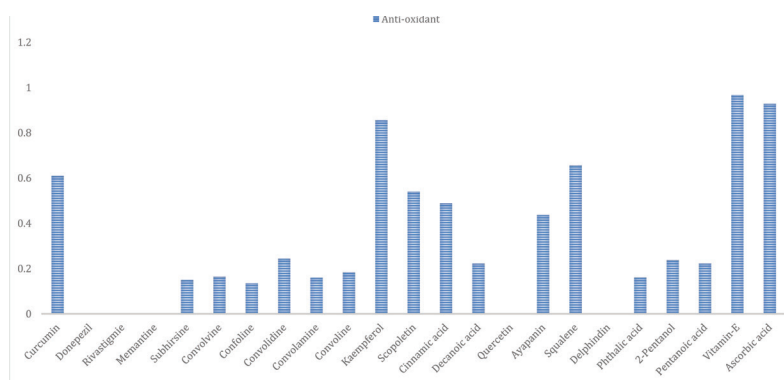


Figure 11: Anti-oxidant activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

Various phytoconstituents are present in *Convolvulus Pluricaulis*, but only a few were explored for their pharmacological activities. Testing every compound by hit and trial method is a very tedious and costly process. But with the help of PASS software, hidden potential activities of phytoconstituents can be explored which was previously not known.

Authorship Contribution

Designing whole manuscript: Sakshi Sharma

Reviewing and guidance: Navneet khurana

Reviewing and editing: Neha Sharma

Literature survey: Vikas Sharma; Soumik Chaudhury

Proofreading: Talluri Sriram; Samriti

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Conflict of interest

There is no conflict of interest.

Declaration

It is an original data and has neither been sent elsewhere nor published anywhere.

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