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# 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


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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. Antiamyloidogenic 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.

| | Pa predicted by PASS software | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Name of compound** | **Reported activity** | **Free radical scavenging activity** | **Dopamine release stimulant** | **Nootropic activity** | **Anti-parkinsonian** | **Catechol O methyl-transferase inhibitor** | **Monoamine oxidase inhibitor** | **Dementia treatment** | **Antia-myloidogenic 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 |

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| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 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 (*Sci-Hub \| Neuro- and Psycho-pharmacological Investigation of the Alkaloids Convolvine and Atropine. Chemistry of Natural Compounds,* 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 |
| Convolidine | 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 |
| Delphindin | 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 > convoline > pentanoic acid = decanoic acid > phthalic acid > convolvine > convolamine > 2-pentanol > subhirsine > confoline.

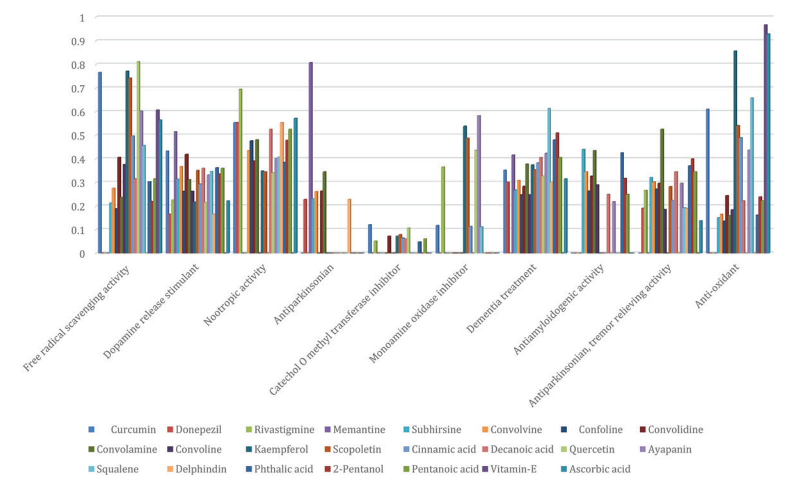


**Figure 1:** All activities of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

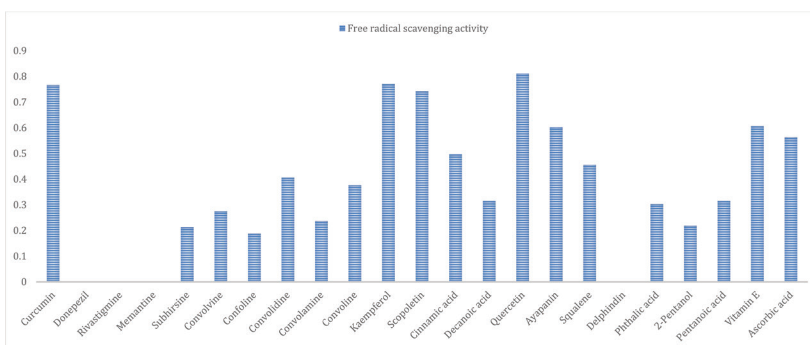


**Figure 2:** Free radical scavenging activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

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 > convoline = confoline > rivastigmine > ascorbic acid > kaempferol > quercetin > donepezil = delphindin.

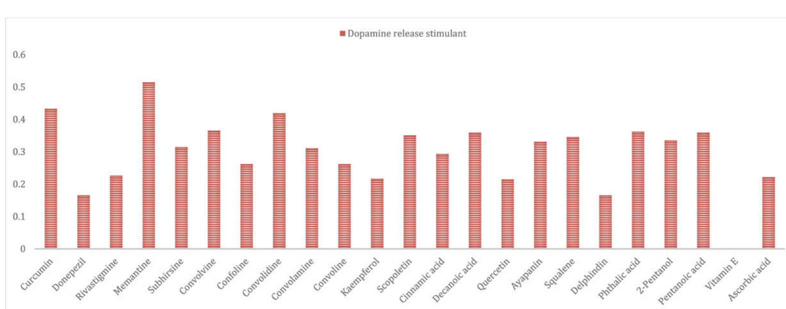


**Figure 3:** Dopamine release stimulant activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

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.

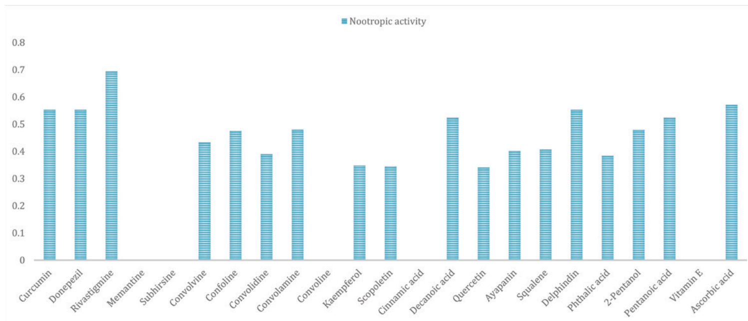


**Figure 4:** Nootropic activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

Only 5 phytoconstituents of CP has shown antiparkinsonian activity (fig. 5) which is as follow: Memantine > convolamine > convolidine > convolvine > subhirsine > donepezil=delphindin.

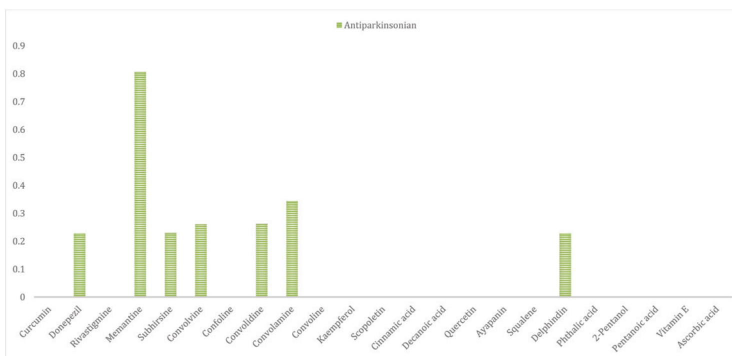


**Figure 5:** Antiparkinsonian activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

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.

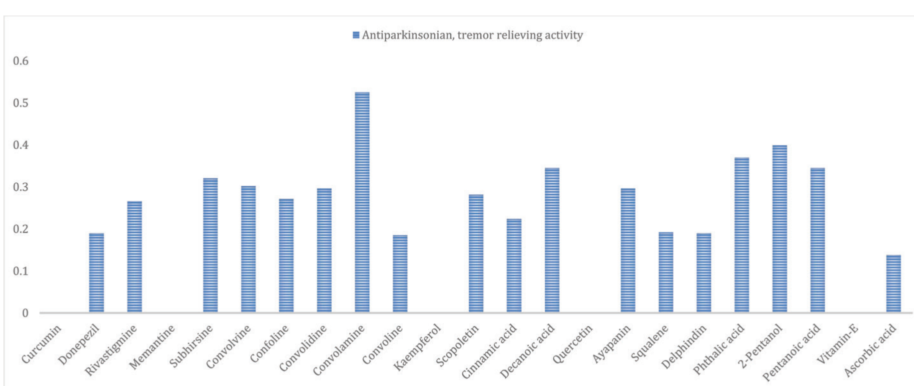


**Figure 6:** Antiparkinsonian, tremor relieving activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

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.

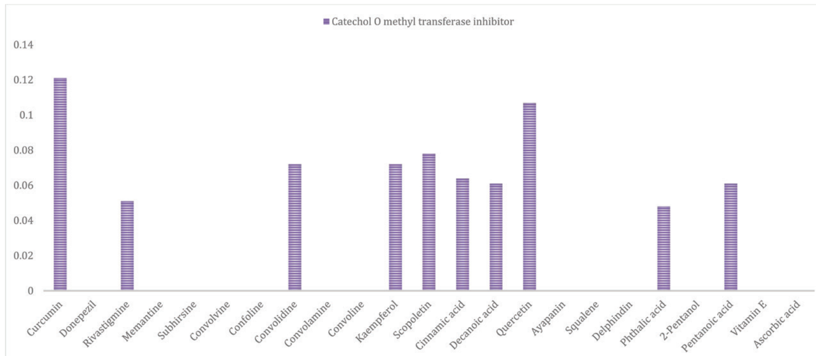


**Figure 7:** COMT inhibitor activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

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 = delphindin > convolidine > subhirsine > convoline > confoline.

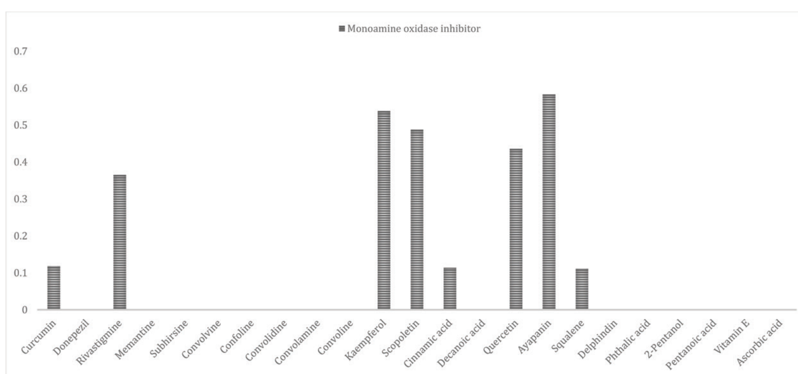


**Figure 8:** MAO inhibitor activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

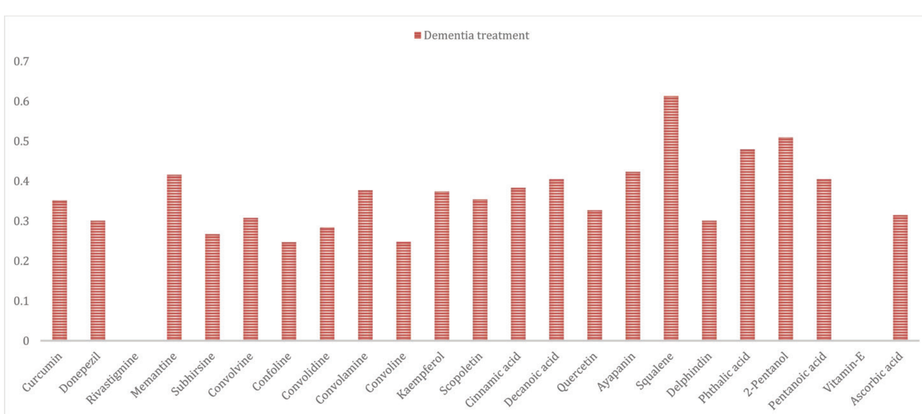


**Figure 9:** Dementia treatment activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

In case of antiamyloidogenic activity eleven phytoconstituents were found to have antiamyloidogenic 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.

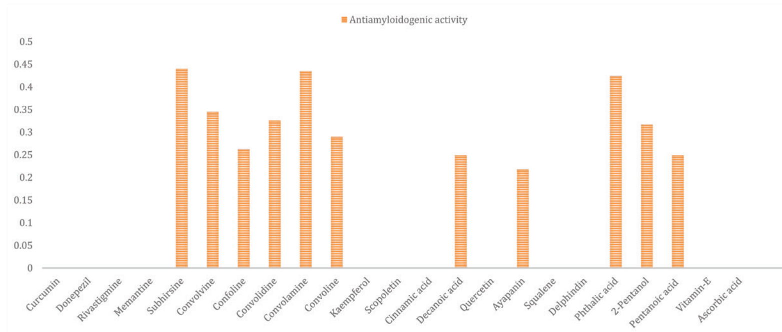


**Figure 10:** Antiamyloidogenic activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

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.

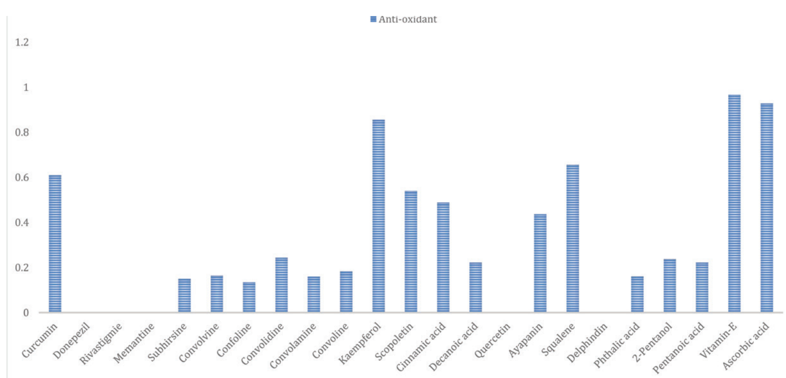


**Figure 11:** Anti-oxidant activity of compounds with respect to Curcumin, Donepezil, Rivastigmine, and Memantine.

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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