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Prediction of the Anti-Parkinson's Effect of Phytoconstituents from *Mucuna Pruriens* with the use of Prediction of Activities Spectra of Substances Software

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ABSTRACT

Mucuna pruriens Linn is the most popular plant which has been used for a long time for treating many diseases. The plants shows wide pharmacological activities like antidiabetic, antineoplastic, antiepileptic, aphrodisiac, antimicrobial activities etc. It has wide use in the treatment of the Parkinson's disease. The rationale behind this study is to discover the maximum activities over the selected phytoconstituent of the plant Mucuna pruriens which can be used in Parkinson's disease. With the help of Prediction of activities spectra of substances (PASS) software activities which are useful in the management of Parkinson's disease can be recognized. The mol file of the compounds was downloaded from Pubchem and the activity of the various compounds was speculated in the PASS software. From the data we have noted the Pa values of the compounds and the related activities of the compounds then we have predicted the reported activities of the compounds and from the table and graph we have observed the higher and lowest value of the compounds showing different activities and also observed which are the compounds which does not show the activities.

1. Introduction

Parkinson's disease is a chronic neurodegenerative disease that primary affects the neurons of the basal ganglia (Rabiei et al., 2019). Parkinson's disease (PD) is classified as the second recurrent neurodegenerative disorder in the whole world and has the twofold rise burden to the former generation(Mozafar et al., 2023). It was first described by the scientist James Parkinson in 1817 The disease cause many symptoms like bradykinesia which is characterized by the delayed initiation and execution of motion, rigidity which is escalated muscle tone, weakened postural reflexes and tremor (Antonini et al., 2017) dyskinesia, non-motor symptoms, quality of life, and safety were evaluated. Observations were fully prospective for treatment-naïve patients (60% of patients. There is attenuation of the pigmented dopaminergic neurons in the substantia nigra, depletion of neurons in the locus coeruleus and atrophic changes in the substantia nigra. Multiple other cell type all over the central and peripheral nervous system are included from the starting of this disease (PANWAR, 2020). Parkinson's disease affects 2-3% of people's population and affects above 65 years age individual. It is mainly begins to the 40 to 70 years individuals. PD under age of 20 is very rare and it is termed as young onset of PD (Savica et al., 2010). It is more seen in man compared to woman. It is mainly associated with non-motor indication that add to altogether disorder (Schapira et al., 2017). The etiology of the Parkinson's disease is not known till date but the factors such as genetics, age, medication and environmental can be responsible for the initiation of this disease (Armstrong & Okun, 2020) a group of neurological disorders with Parkinson disease-like movement problems such as rigidity, slowness, and tremor. More than 6 million individuals worldwide have Parkinson disease. Observations: Diagnosis of Parkinson disease is based on history and examination. History can include prodromal features (eg, rapid eye movement sleep behavior disorder, hyposmia, constipation. Insufficient improvement from the accelerating development of the disease has been regarded to consequences from the basal clinical degeneration revealed by inducing agent (Calzetti & Negrotti, 2023). The pharmacotherapy available for the cure of the underline cause of PD is Levodopa and Carbidopa. These drugs also produces various side effects like vomiting, nausea, convulsions, dry mouth and hallucinations (Olanow et al., 2009).

From the ancient time herbal medicine has been used in the treatment of various disease symptoms. Now days with the recent advancement of the technology we can assess the phytoconstituent present in all the plants and that can be used for the various pharmacological treatments. The phytoconstituent will determine the overall usage and nature of the plant. Numerous plants used in the management of the Parkinson's disease are *Mucuna pruriens* (Katzenshlager

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et al., 2004), Paeonia suffruticosa, Hyoscyamus niger seeds, Hibiscus asper leaves etc. It was seen that *Mucuna pruriens* comprises of high levels of levodopa which is the one of the main pharmacotherapy of Parkinson's disease (*High Levels of Levodopa Found in Mucuna Pruriens Supplements | Mucuna Pruriens Supplements May Lead to Excess Levodopa in Patients | Parkinson's News Today*, n.d.). *Mucuna pruriens* also attenuates the motor symptoms of the Parkinson's disease and some studies suggested that single dose of the *Mucuna pruriens* has the quick onset as well as the extended action comparative to the normal pharmacotherapy of the Parkinson's disease by decreasing side effects like dyskinesis (*Science of Mucuna Pruriens for Treating Parkinson's | APDA*, n.d.). The drugs can be obtained from the different parts of the plants like bark, leaves, stem, seeds, pods and including flower also(*(PDF) Phytochemistry and Pharmacological Activity of Mucuna Pruriens: A Review*, n.d.). Many plants are experimented in the in vivo and in vitro (*(PDF) In Vitro Evaluation of the Antibacterial Activity of Mucuna Pruriens Leaf and Callus Extracts*, n.d.) conditions (Lampariello et al., 2012). Various phytochemicals like Levodopa (Pathania et al., 2020), Beta carboline, Gallic acid, Glutamic acid, Cysteine, Docosonoic acid, 6-methoxy tryptamine, Serotonin, Genistoside, l-proline, Nicotine, Tryptamine, Oleic acid, Squalene, Lenoleic acid, Stearic acid, Palmitic acid, l-leucine, Bufotenine, Ascorbic acid, 5-hydroxytryptophan, 3-carboxysalsolinol, Isoharmine, N,N-Dimethyl tryptamine, Quinolone, l-phenylalanine, l-lysine exhibits numerous activities that are useful in the management of the Parkinson's disease (*(PDF) Review on "Mucuna" - The Wonder Plant*, n.d.). The overall activities of all these components has been scrutinized and various prognosis are evaluated that are useful in the management of the Parkinson's disease(Tavares et al., 2020). Hence the budgetary use of remedial plants are escalating day by day and abundant investigations are conducting for various plants for inspecting the numerous activities and in the latest times many other tactics and other prophecies will be inspected which are found to be useful in the treatment of Parkinson's disease(P. Kumar & Saha, 2013). Nevertheless the efficacy and safety of all the phytochemicals should be farther more estimated so that it can be used for the safe use in managing various disease like Parkinson's disease (Farnsworth et al., 1985).

Chemical constituents: Levodopa(*Levodopa*, n.d.), Beta carboline, Gallic acid (Badhani et al., 2015), Glutamic acid, Cysteine, Docosonoic acid, 6-methoxy tryptamine, Serotonin(*Serotonin*, n.d.), Genistoside, l-proline, Nicotine, Tryptamine, Stearic acid(*Stearic Acid*, n.d.), Squalene(*Squalene*, n.d.), Palmitic acid (Voon et al., 2011) but its effects on plasma homocysteine and inflammatory markers are unclear. Objective: We investigated the effects of high-protein Malaysian diets prepared with palm olein, coconut oil (CO, Oleic acid (Lopez et al., 2010), Linoleic acid (Johnson & Fritsche, 2012), l-leucine, Bufotenine (*Bufotenin Oxide | C12H16N2O2 - PubChem*, n.d.), Ascorbic acid (Charleston & Clegg, 1972), 5-hydroxytryptophan(*5-Hydroxy Tryptophan*, n.d.), 3-carboxysalsolinol, Isoharmine, N,N-Dimethyl tryptamine (James et al., 2022)addictions, post-traumatic stress disorder, anxiety and specific psychoneuroendocrine immune system pathologies. The article assesses potential ayahuasca and N,N-dimethyltryptamine (DMT, Quinolone, l-phenylalanine, l-lysine.

2. Methods

The activities of the various phytoconstituents, which helps in managing Parkinson's disease, present in the *Mucuna pruriens* can be estimated with the help of Prediction of activities spectra of substances (PASS) software (R. Kumar et al., 2018). In this software, the activities are estimated in the terms of two probabilities; that is Pa (probable activity) and Pi (probable inactivity). The value of Pa and Pi varies from 0.000 to 1.000. The activities with Pa > Pi are only selected for any compound. The Probable activity values higher than 0.7 has more probability of higher pharmacological actions. The Probable activity values lower than 0.5 has lesser pharmacological actions. The compounds with Probable activity more than 0.5 and less than 0.7 have the less probability of being effective in various pharmacological investigations (Lagunin et al., 2000).

The PASS Software is used for investigating various effects of the compounds (Poroikov et al., 2003). Here the phytochemicals with the reported pharmacological actions that are useful in managing the Parkinson's disease are being selected. For the estimation of the activities we have inspected the various actions of the components by entering the MOL file of the compound that is prevailed from Pubchem website. The activities of the compounds can also assessed by putting the (SMILES) Simplified Molecular-Input-Line-Entry System in the PASS software. These SMILES are working as a molecular formula, by putting it the overall data of the phytochemicals is revealed. The Probable activity and the Probable inactivity values are unveiled and the estimated activities are described here. Thus the activities of various phytochemicals are investigated by the help of PASS software. These activities are farther evaluated and can be used for management of the disease like Parkinson's disease.

Results

The activities of the selected phytochemicals were anticipated by the help of PASS software.

The compounds like Levodopa, Beta carboline, Gallic acid, Glutamic acid, Cysteine, Docosonoic acid, 6-methoxy tryptamine, Serotonin, Genistoside, l-proline, Nicotine, Tryptamine, Linoleic acid, Squalene, Palmitic acid, Stearic acid, Oliec acid, l-leucine, Bufotenine, Ascorbic acid, 5-hydroxytryptophan, 3-carboxysalsolinol, Isoharmine, N,N-Dimethyl tryptamine, Quinolone, l-phenylalanine, l-lysine shows these activities as follows (Tan et al., 2009) (*MUCUNA PRURIENS SHOWS NEUROPROTECTIVE EFFECT BY INHIBITING APOPTOTIC PATHWAYS OF DOPAMINERGIC NEURONS IN THE PARAQUAT MOUSE MODEL OF PARKINSONISM | Request PDF*, n.d.).

- Dopamine release stimulant
- Antiparkinsonian, tremor relieving
- Antiparkinsonian, rigidity relieving
- Dopa decarboxylase inhibitor
- MAO inhibitor
- Free radical scavenger
- Catechol O Methyl transferase inhibitor
- NMDA receptor antagonist

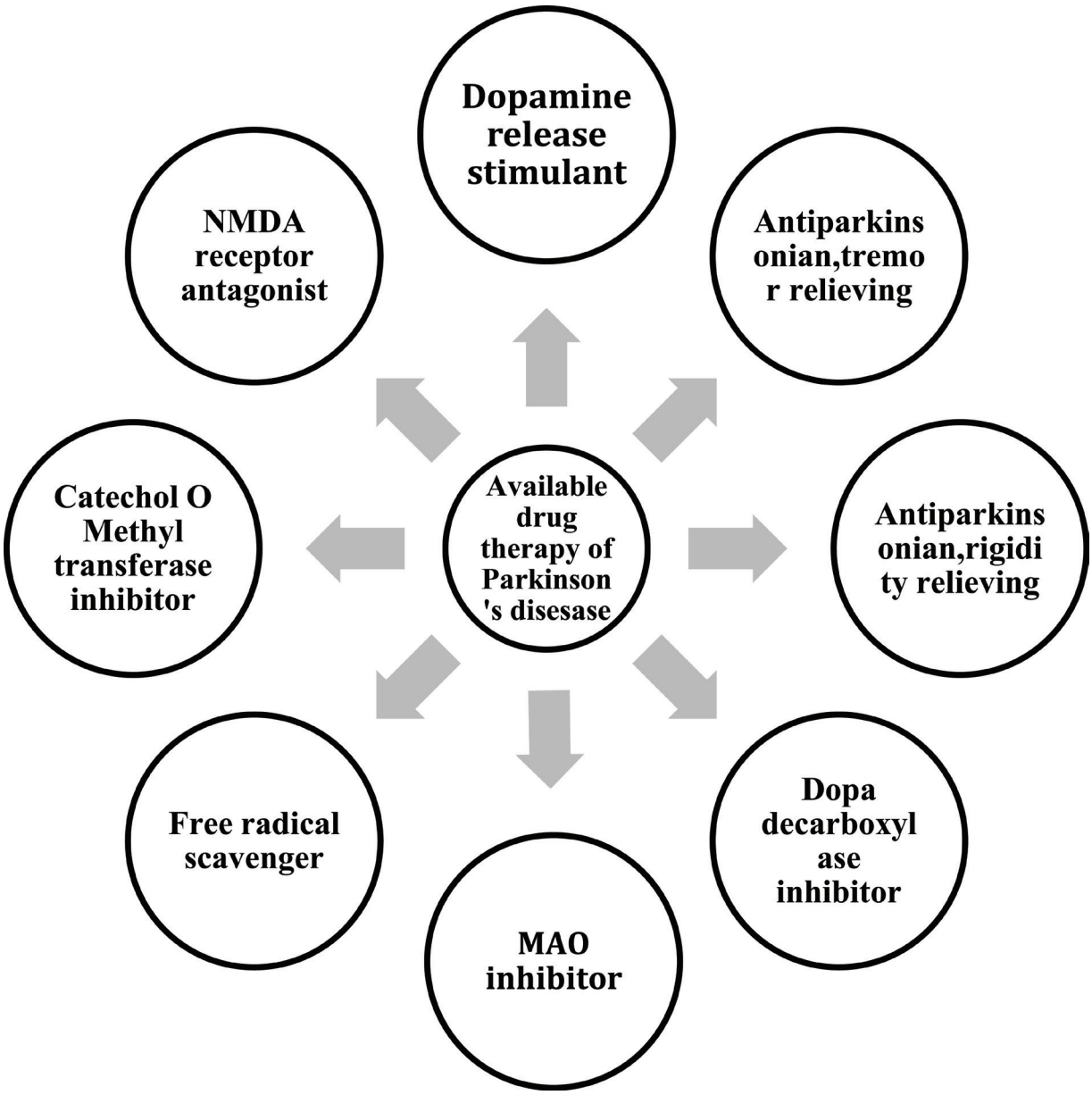
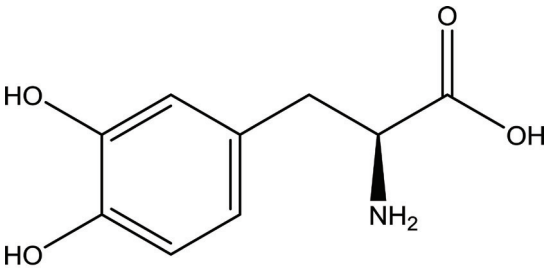
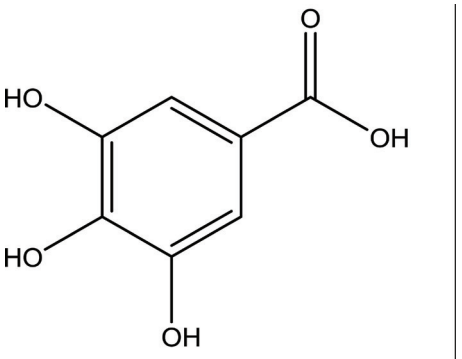
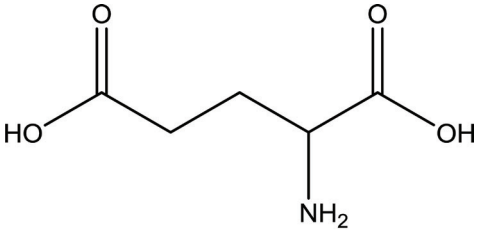
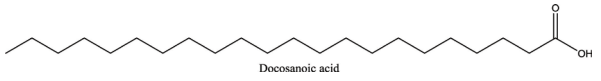
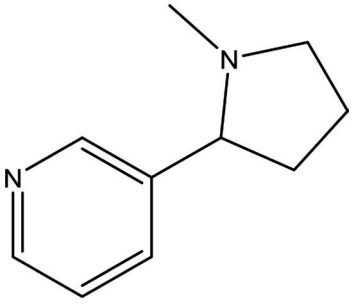
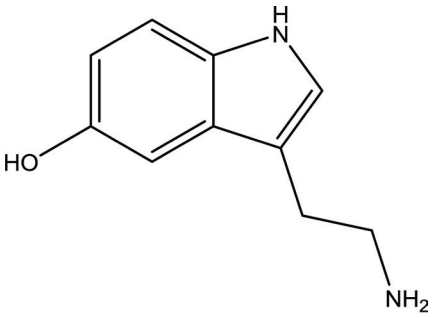
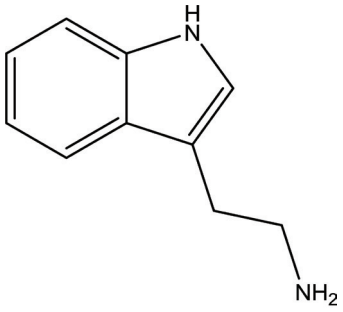
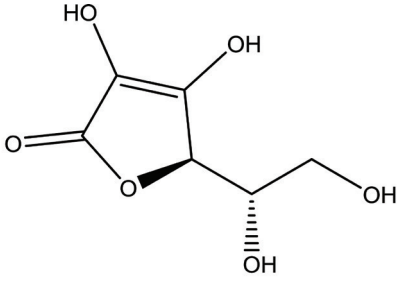
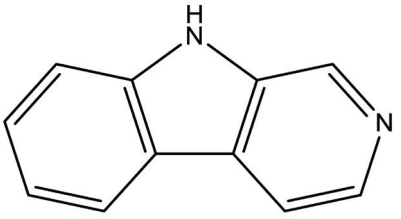
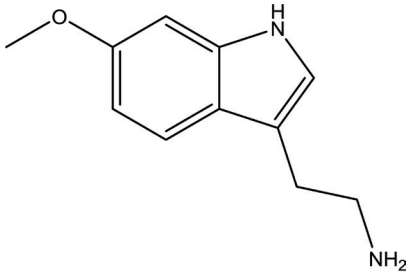
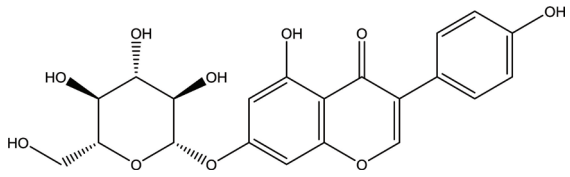
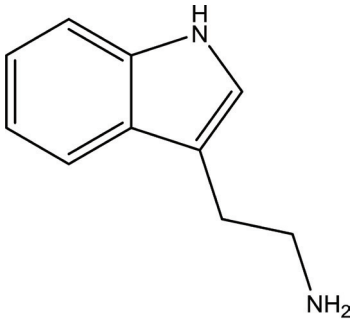
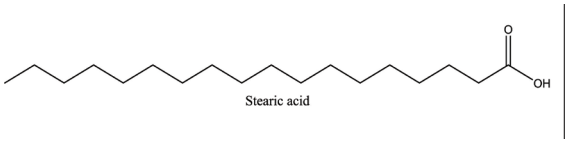
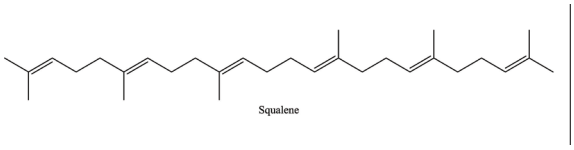
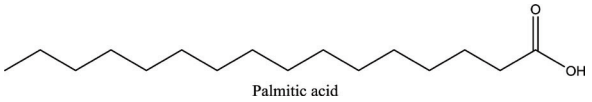
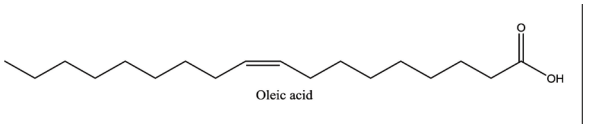
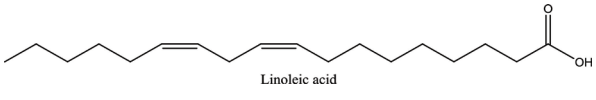
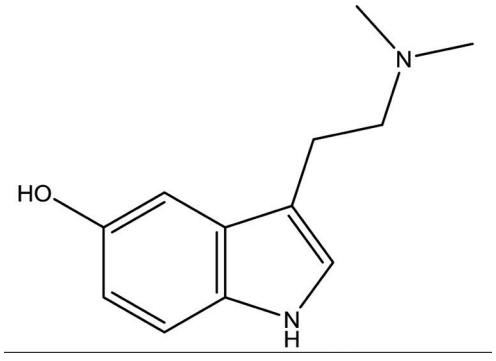


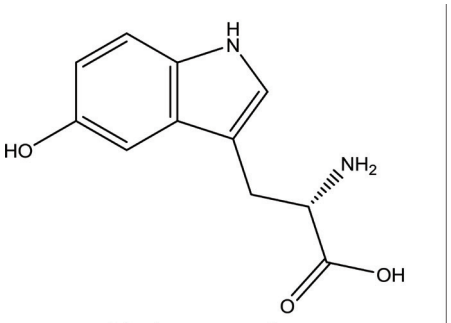
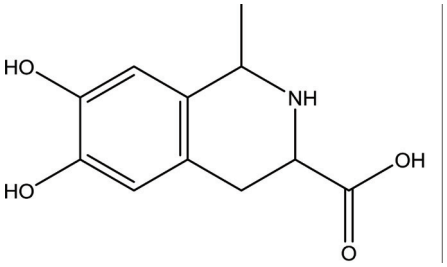
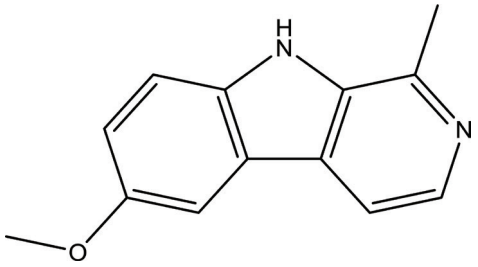
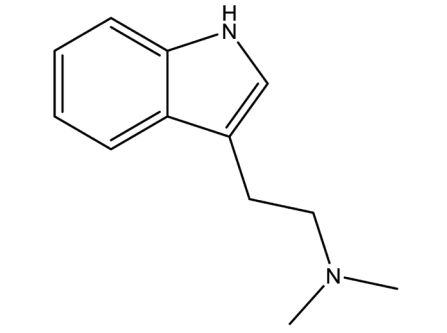
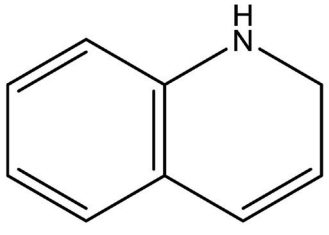
Figure: Available pharmacotherapy for Parkinson's disease.

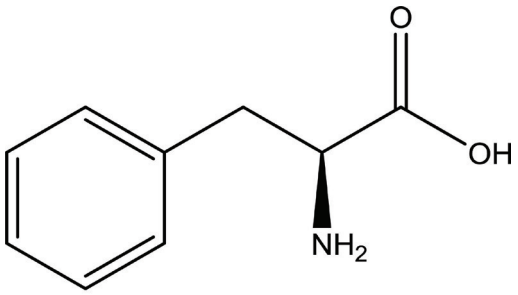
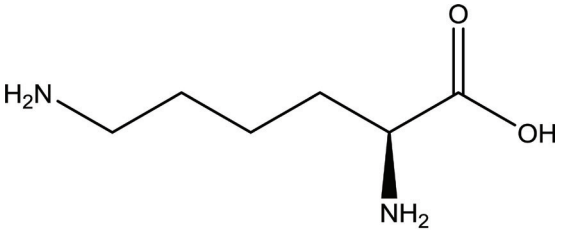
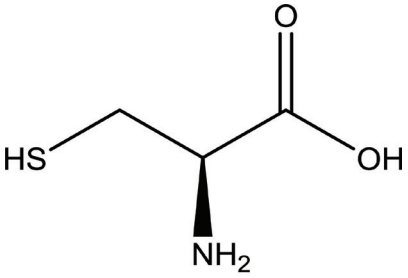
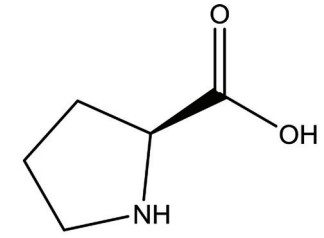
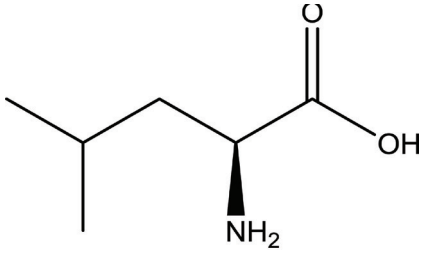
Table Phytoconstituents name and their chemical structures

Name of compound	**Structures**
Levodopa	 3-hydroxy-L-tyrosine
Gallic acid	 3,4,5-Trihydroxybenzoic Acid Acid
Glutamic acid	 2-Aminopentanedioic acid
Docosonoic acid	 Docosanoic acid
Nicotine	 nicotine

Serotonin	 serotonin
Tryptamine	 tryptamine
Ascorbic acid	 ascorbic acid
Beta carboline	 beta-carboline
6-methoxytryptamine	 6-methoxytryptamine

Genistoside	
Tryptamine	 Tryptamine
Stearic acid	 Stearic acid
Squalene	 Squalene
Palmitic acid	 Palmitic acid
Oleic acid	 Oleic acid
Linoleic acid	 Linoleic acid
Bufotenine	

5-hydroxytryptophan	 5-hydroxytryptophan
3-Carboxysalsolinol	
Isoharmine	
N,N-dimethyltryptamine	 N,N-dimethyltryptamine
Quinolone	 Quinolone

L-phenylalanine	 L-phenylalanine
L-lysine	 L-lysine
Cysteine	 Cysteine
L-proline	 L-proline
L-leucine	 L-leucine

Pa PREDICTED BY PASS SOFTWARE									
Name of compound	Reported activity	Dopamine release stimulant	Dopa decarboxylase inhibitor	Anti-parkinsonian, rigidity relieving	Anti-parkinsonian, tremor relieving	Free radical scavenger	MAO inhibitor	Catechol O Methyl transferase inhibitor	NMDA receptor antagonist
Levodopa	DA Agonist (Katzenschlager & Lees, 2002)	0.547	0.824	0.221	0.304	0.377	0.095	0.087	0.167
Beta carboline	N-methylation (Matsubara et al., 2002)	0.169	0.159	0.236	0.147	NP	NP	NP	0.072
Gallic acid	Increases life span and loco motor activity (Ortega-Arellano et al., 2013)	0.422	NP	0.284	0.373	0.57	NP	0.188	0.117
Glutamic acid	Decreased glutamic acid decarboxylase mRNA expression (Lanoue et al., 2010)	0.358	0.518	0.272	0.242	0.286	NP	NP	0.131
Cysteine	Reduction of dopaminergic neuronal degeneration (Martínez-Banaclocha, 2012)	0.377	0.482	0.26	0.236	0.375	NP	NP	NP
Docosonoic acid	improved motor performance and less dopaminergic degeneration (Metzdorf & Tönges, 2021)	0.36	0.35	0.432	0.345	0.315	NP	0.061	0.07
6-methoxy tryptamine	Neuroprotective effect (Mack et al., 2016)	0.23	0.301	NP	0.306	0.252	0.128	NP	NP
Serotonin	Induce dyskinesia (Iderberg et al., 2015)	0.21	0.537	0.218	0.32	0.318	0.111	NP	0.116
Genistoside	NR	NP	0.42	NP	NP	0.791	0.196	NP	NP
l-proline	Neuroprotective effect (Misiura & Miltyk, 2019)	0.35	0.278	0.539	0.418	0.154	NP	NP	0.399
Nicotine	Increase DAT level (Quik et al., 2006)	0.213	NP	0.427	0.407	NP	NP	NP	NP

Tryptamine	endogenous enhancer substance (Shimazu & Miklya, 2004)	0.192	0.369	0.39	0.412	0.196	0.099	NP	0.088
Stearic acid	Improves survival and mitochondrial functions (Bajracharya et al., 2019)	0.36	0.35	0.432	0.345	0.315	NP	0.061	0.07
Squalene	Increases oxidative damage in the striatum (Kabuto et al., 2013)	0.346	0.187	0.321	0.192	0.456	0.111	NP	NP
Palmitic acid	increase in α-syn and tyrosine hydroxylase protein and mRNA expression levels (Schommer et al., 2018)	0.36	0.35	0.432	0.345	0.315	NP	0.061	0.07
Oleic acid	Neuroprotective role (Ubaid et al., 2020)	0.278	0.263	0.359	0.339	0.36	NP	0.048	NP
Linoleic acid	normal cellular function (Youdim et al., 2000)	0.256	0.235	0.323	0.304	0.315	NP	NP	NP
l-leucine	LRRK2 has role in pathogenesis of idiopathic PD (Tolosa et al., 2020)	0.341	0.477	0.441	0.33	0.288	NP	NP	NP
Bufotenine	Psychotropic effects (Takeda, 1994)	0.206	0.374	0.341	0.408	0.341	0.118	NP	0.071
Ascorbic acid	Reduce levodopa dosage without losing its effectiveness (Nagayama et al., 2004)	0.222	0.2	NP	0.138	0.564	NP	NP	NP
5-hydro-xytryptophan	Treating depressive symptoms (Meloni et al., 2020)	0.199	0.818	NP	0.225	0.304	NP	NP	0.152
3-carbo xysalsolinol	NR	0.261	0.387	0.187	0.208	0.21	NP	0.051	0.247
Isoharmine	NR	0.188	NP	NP	0.147	0.201	0.227	NP	NP
N,N-Dimethyl tryptamine	NR	0.189	0.209	0.513	0.508	0.206	0.107	NP	NP

Quinolone	Neuroprotective (Kim, 2010)	0.222	0.201	0.319	0.219	0.163	0.121	NP	NP
l-phenylalanine	Activation of dopamine synthesis (Ishikawa et al., 2009)	0.44	0.707	0.36	0.414	0.231	0.106	NP	0.197
l-lysine	Imbalance of lysine acetylation contributes to pathogenesis of PD (Wang et al., 2020)	0.31	0.41	0.258	0.286	0.281	NP	NP	0.168

PD- Parkinson's disease, DAT- Dopamine transporter, DA- Dopamine agonist, LRRK2-leucine-rich repeat kinase 2, NR- Not Reported, NP- Not Predicted

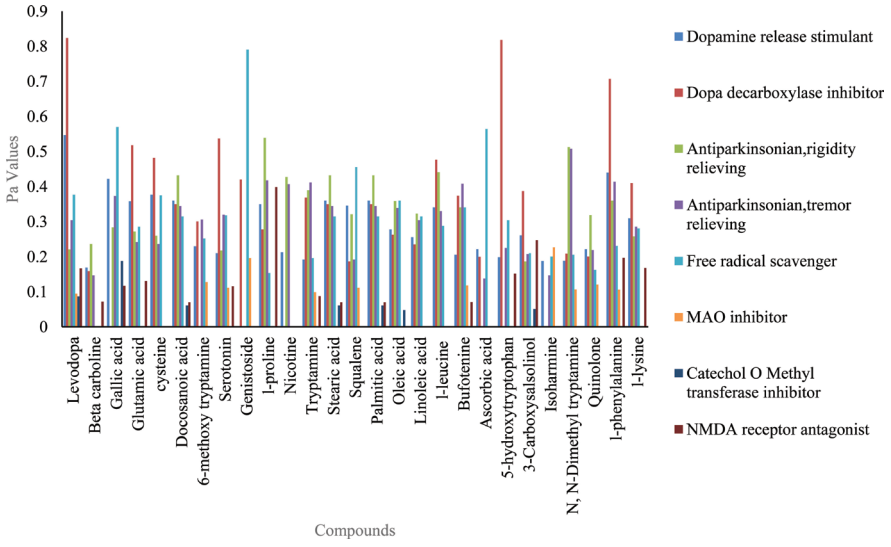


Figure 1: Activities of all the compounds with reference to levodopa.

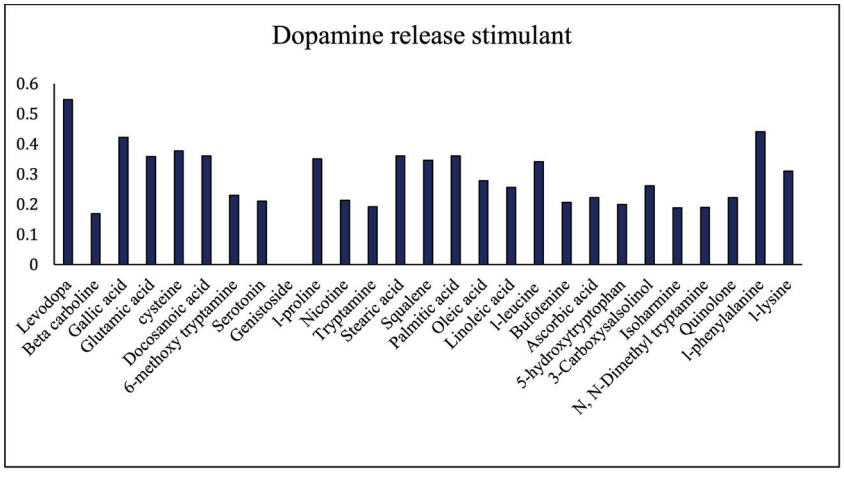


Figure 2: Dopamine release stimulant activity of all compound with reference to levodopa.

The phytochemicals exhibiting Dopamine release stimulant activity follows the pattern:-

Levodopa > l-phenylalanine > Gallic acid > Cysteine > Docosonoic acid > Stearic acid > Palmitic acid > l-proline > Glutamic acid > Squalene> l-leucine > l-lysine >Oleic acid > 3-carboxysalsolinol > Linoleic acid > 6-methoxy tryptamine > Ascorbic acid > Quinolone > Nicotine > Serotonin > Bufotenine > 5-hydroxytryptophan > Tryptamine > N, N-Dimethyl tryptamine > Isoharmine > Beta carboline

It was seen that Levodopa is having high value for Dopamine release stimulant activity and Beta carboline is having less value. Genistoside does not show Dopamine release stimulant activity.

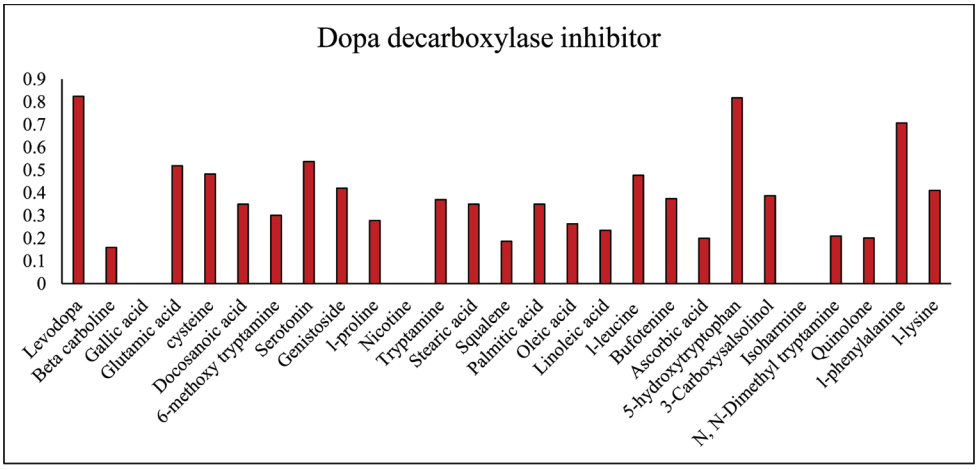


Figure 3: Dopa decarboxylase inhibitor activity of all compounds with reference to levodopa.

The phytochemicals exhibiting Dopa decarboxylase inhibitor activity follows the pattern:-

Levodopa > 5-hydroxytryptophan > l-phenylalanine > Serotonin > Glutamic acid > cysteine > L-leucine > Genistoside > L-lysine > 3-carboxysalsolinol > Bufotenine > Tryptamine > Palmitic acid > Stearic acid > Docosanoic acid > 6-methoxy tryptamine > L-proline > Oleic acid > Linoleic acid > N, N-Dimethyl tryptamine > Quinolone > Ascorbic acid > Squalene > Beta carboline

It was seen that Levodopa is having high value for Dopa decarboxylase inhibitor activity and Beta carboline is having less value. Gallic acid, Nicotine, Isoharmine does not show Dopa decarboxylase inhibitor activity.

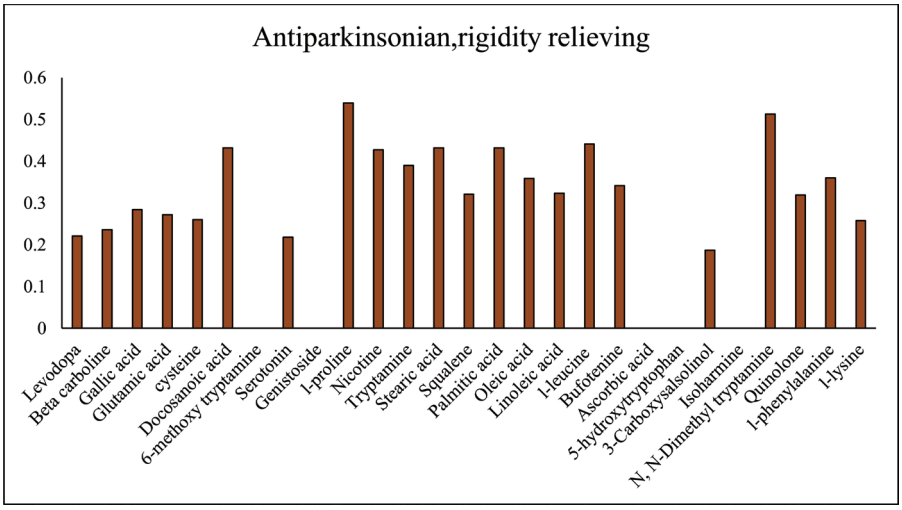


Figure 4: Antiparkinsonian, rigidity alleviating activity of all compound with reference to levodopa.

The phytochemicals exhibiting Antiparkinsonian, rigidity alleviating activity follows the pattern:-

L-proline > N, N-Dimethyl tryptamine > L-leucine > Docosanoic acid > Palmitic acid > Stearic acid > Nicotine > Tryptamine > L-phenylalanine > Oleic acid > Bufotenine > Linoleic acid > Quinolone > Squalene > Gallic acid > Glutamic acid > Cysteine > l-lysine > Beta carboline > Levodopa > Serotonin > 3-carboxysalsolinol

We have found that l-proline shows higher values for Antiparkinsonian, rigidity relieving activity and 3-carboxysalsolinol shows least value. 6-methoxy tryptamine, Genistoside, Ascorbic acid, 5-hydroxytryptophan and Isoharmine does not show any activity for Antiparkinsonian, rigidity relieving activity.

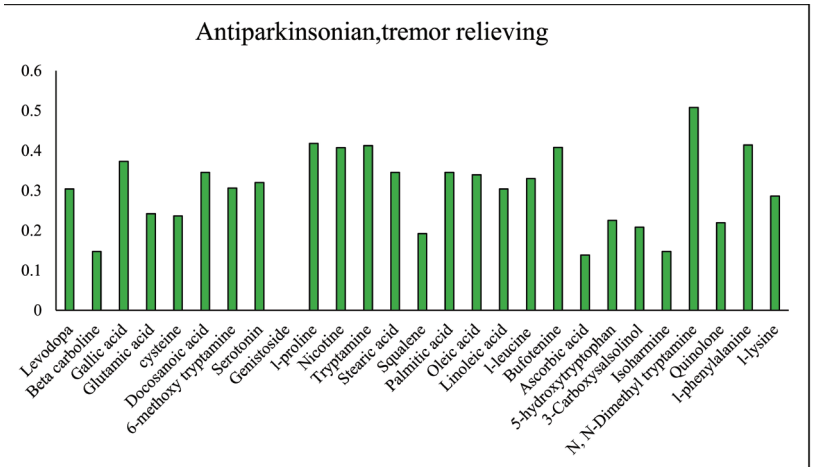


Figure 5: Antiparkinsonian, tremor relieving activity of all compound with reference to levodopa.

The phytochemicals exhibiting Antiparkinsonian, tremor relieving activity follows the pattern:-

N, N-Dimethyl tryptamine > L-proline > L-phenylalanine > Tryptamine > Bufotenine > Nicotine > Gallic acid > Stearic acid > Docosanoic acid > Palmitic acid > Oleic acid > L-leucine > Serotonin > 6-methoxytryptamine > Levodopa > Linoleic acid > L-lysine > Glutamic acid > Cysteine > 5-Hydroxytryptaphan > Quinolone > 3-Carboxysalsolinol > Squalene > Beta carboline > Isoharmine > Ascorbic acid

We have found that N, N-Dimethyl tryptamine shows higher value for Antiparkinsonian, tremor relieving activity and Ascorbic acid shows least value. Genistoside, does not show any activity for Antiparkinsonian, tremor relieving.

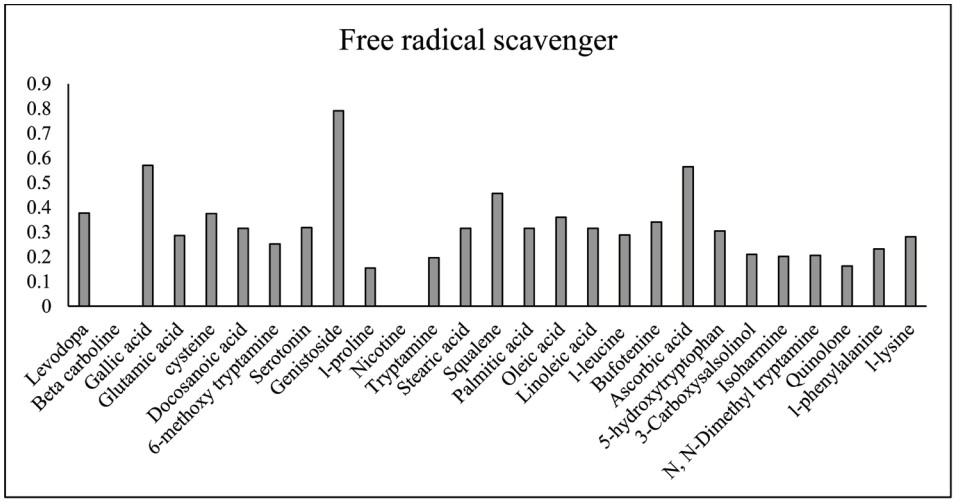


Figure 6: Free radical scavenger activity of all compounds with reference to ascorbic acid.

The phytochemicals exhibiting free radical scavenger activity follows the pattern:-

Genistoside > Gallic acid > Ascorbic acid > Squalene > Levodopa > Cysteine > Oleic acid > Bufotenine > Serotonin > Docosanoic acid > Stearic acid > Linoleic acid > Palmitic acid > 5-Hydroxytryptophan > L-leucine > Glutamic acid > L-lysine > 6-methoxy tryptamine > L-phenylalanine > 3-carboxysalsolinol > N, N-Dimethyl tryptamine > Isoharmine > Tryptamine > Quinolone > L-proline

From the graph we witnessed that Genistoside is showing higher value for Free radical scavenger activity and l-proline shows least value. Beta carboline and Nicotine does not exhibits Free radical scavenger activity.

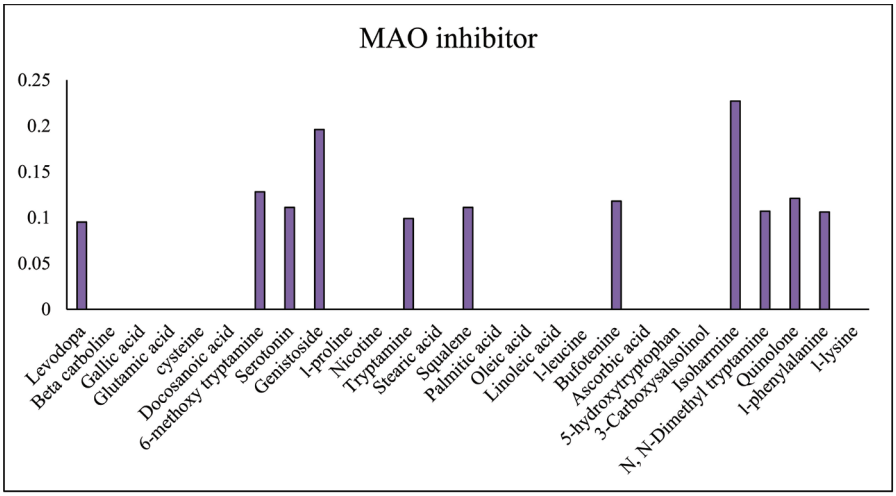


Figure 7: MAO inhibitor activity of all compounds with reference to selaginin.

The phytochemicals exhibiting MAO inhibitor activity follows the pattern:-

Isoharmine > Genistoside > 6-methoxy tryptamine > Quinolone > Bufotenine > Squalene > Serotonin > N, N-Dimethyl tryptamine > l-phenylalanine > Tryptamine > Levodopa We have found that Isoharmine shows higher value for MAO inhibitor activity and Levodopa shows least activity.

Beta carboline, Gallic acid, Glutamic acid, Cysteine, Docosanoic acid, l-proline, Nicotine, Oleic acid, Linoleic acid, Plamitic acid, Stearic acid, l-leucine, Ascorbic acid, 5-hydroxytryptophan, 3-carboxysalsolinol and l-lysine does not show MAO inhibitor activity.

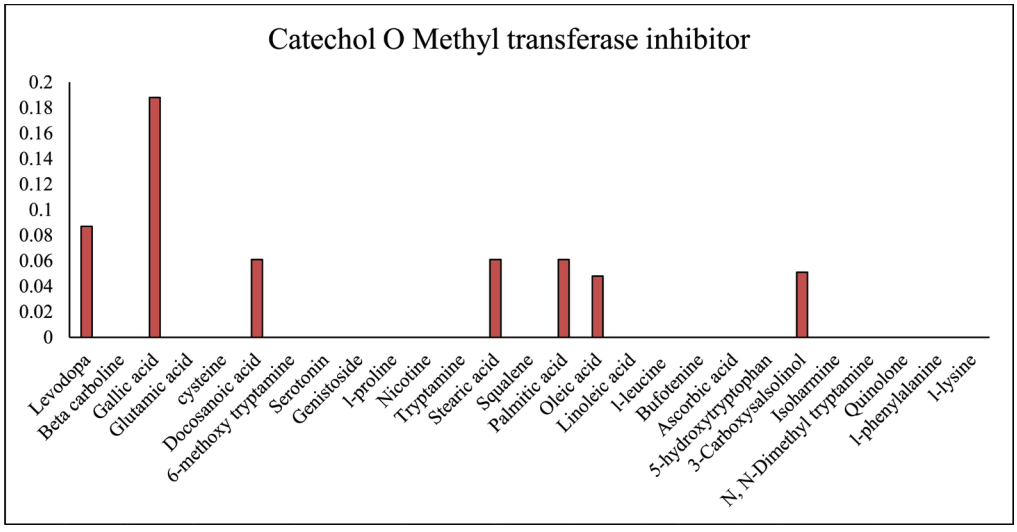


Figure 8: Catechol O Methyl transferase inhibitor activity of all compounds with reference to entacapone.

The phytochemicals exhibiting Catechol O Methyl transferase inhibitor activity follows the pattern:-

Gallic acid > Levodopa > Docosanoic acid > Stearic acid > Palmitic acid > 3-Carboxysalsolinol > Oleic acid

We have found that Gallic acid shows higher value for Catechol O Methyl transferase inhibitor activity and Oleic acid shows least value. Beta carboline, Glutamic acid, Cysteine, 6-methoxy tryptamine, Serotonin, Genistoside, l-proline, Nicotine, Tryptamine, Squalene, Linoleic acid, l-leucine, Bufotenine, Ascorbic acid, 5-hydroxytryptophan, Isoharmine, N, N-Dimethyl tryptamine, Quinolone, l-phenylalanine and l-lysine does not show Catechol O Methyl transferase inhibitor activity.

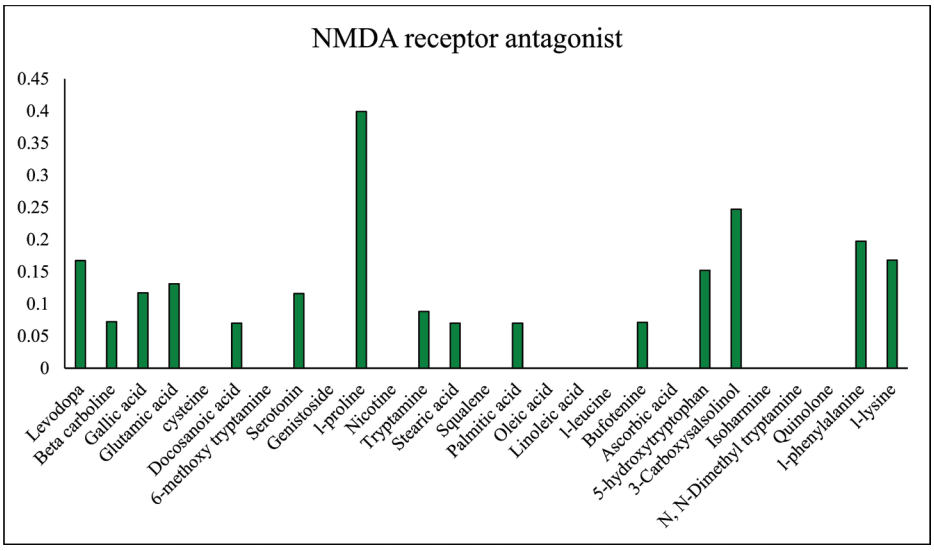


Figure 9: NMDA receptor antagonistic activity of all compounds with reference to amantadine.

The phytochemicals exhibiting NMDA receptor antagonistic activity follows the pattern:-

L-proline > 3-carboxysalsolinol > l-phenylalanine > l-lysine > 5-hydroxytryptophan > Levodopa > Glutamic acid > Gallic acid > Serotonin > Tryptamine > Beta carboline > Bufotenine > Docosanoic acid > Stearic acid > Palmitic acid

We have found that L-proline shows higher value for NMDA receptor antagonist activity and Palmitic acid shows least value.

Cysteine, 6-methoxy tryptamine, Genistoside, Nicotine, Squalene, Oleic acid, Linoleic acid, l-leucine, Ascorbic acid, Isoharmine, N, N-Dimethyl tryptamine and Quinolone does not show NMDA receptor antagonist activity.

Conclusion

It is concluded from our study that PASS software forks out the data that provides the information to hold up the reported activities of the phytochemicals. From this study we have inspected the reported activity of all the phytochemicals and their reported effect in the management of Parkinson's disease. From this study we have anticipated the activities of all the phytochemicals which can be used in treating Parkinson's disease.

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

Funding

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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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