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Creation And Designing Of PENN Database For Natural Molecules Effective Against Age Related Disorders

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Abstract

PENN Database (**P**lant **E**xtracted **N**atural molecules for **N**eurodegeneration) is online database (www.penndatabase.info) dedicated to various neurodegenerative disorders such as Parkinson's, Alzheimer's, Huntington's, Amyotrophic lateral sclerosis and Creutzfeldt Jacob's and several natural molecules known to prevent and/or cure these age related diseases. To each of the natural molecules link for pubchem and pubmed is provided through respective CIDs and PMIDs. Mysql was used for designing and creation of the database while the language of programming applied for creating the database is php. Further, web page designing and online accessibility of database is accomplished by html and css. The PENN database provides links for details of individual molecules making it a useful and versatile online tool. The information in the database could be exploited for designing of experiments to study comparative effects of natural molecules on neurodegenerative diseases.

Keywords: *Protein misfolding disorder, Database, Natural molecule, Mysql, php scripting language*

Introduction

Age related neurodegenerative diseases such as Alzheimer's disease (AD), Parkinson's disease (PD), Huntington's, Amyotrophic lateral sclerosis (ALS), and neuron infectious disease such as Creutzfeldt Jacob's are increasing in prevalence with population in most countries across the globe. Their molecular mechanism of these disorders share similar pathologies [1]. The key pathological features playing a central role in these disorder are misfolding and aggregation of protein such as α-synuclein (α-syn) in Parkinson's disease (PD), β-amyloid in Alzheimer's disease and prions (prp) in transmissible spongiform encephalopathies (TSEs). The accumulation of misfolded protein aggregates triggers various unfolded-protein responses or UPRs [2] and imposes stress on ER as the protein maturation and processing in the cell occurs in ER [3]. This results in overall disturbances in the normal functioning of the cells leading to complex cascade of clinical events such as saturation of the proteasome system and activation of apoptotic pathways [4]. Currently, PMDs include >25 clinically diverse human and animal disorders . The issues related to only symptomatic treatments have been addressed till date, with no solution for cure or progression of the disorders. Thus, in the present context, there is an urgent need for a new bio-chemical entity(s) with zero or low toxicity, which can effectively act on diverse molecular targets of PMDs. The abundant natural molecules of plant origin and their modification have yielded not only the new lead molecules for drug discovery and development but also the nutraceuticals [5].

The various sources of catechin and their mechanism of action in protection against neurodegeneration are reviewed extensively [6]. The presence of catechols and their derivative obtained from *Withania somnifera* effected the neural growth and locomotion in in-vivo Parkinson's diseased mouse models [7]. In vivo tests have been carried out on mice models to study the role of Curcumin and their derivatives from *Curcuma longa* in learning and spatial memory with respect to Neurodegeneration [8].

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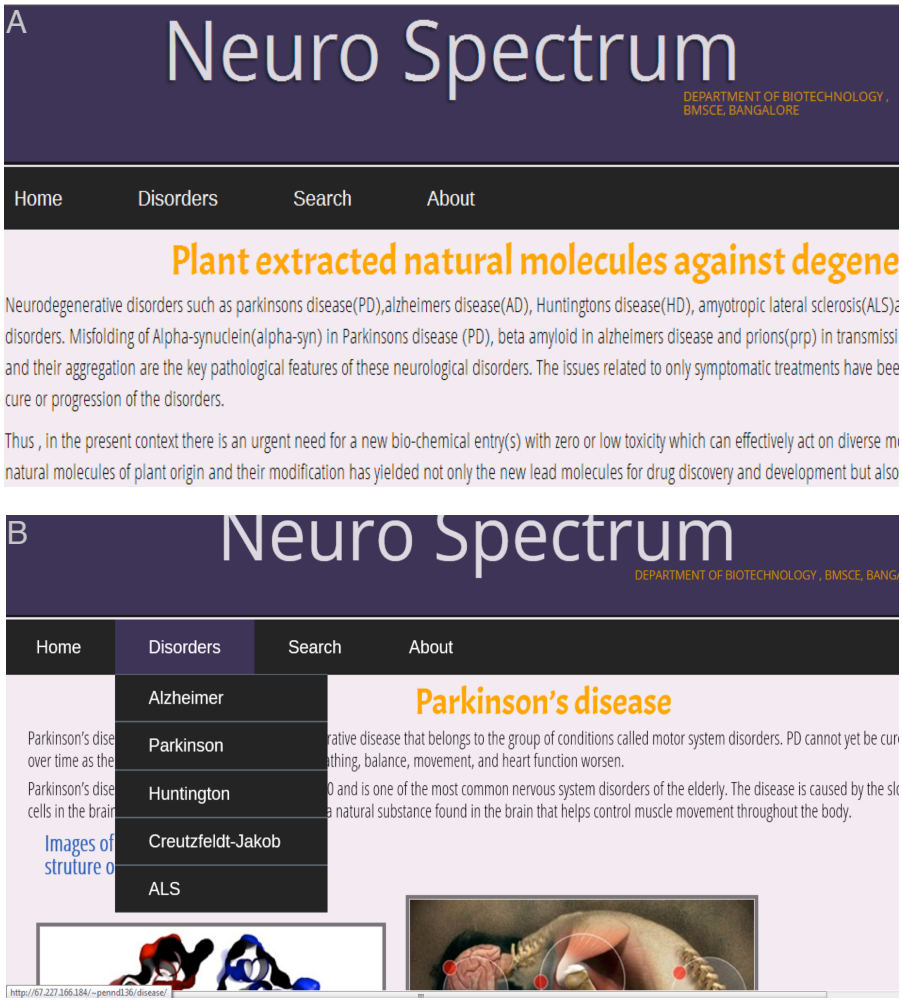
The present work is aimed towards creating a database (www.penndatabase.info) comprising of information for both neurodegenerative diseases and natural molecules obtained from plants known to cure/prevent these diseases.

Methods

The data on the symptoms, causes, diagnosis, molecular basis, drugs available for treatment of Parkinson's, Alzheimer's, Huntington's, Amyotrophic lateral sclerosis and Creutzfeldt Jacob's neurodegenerative disorders were collected from published articles and public databases such as PDB, KEGG and NCBI. Similarly plant extracted natural molecules known to treat/prevent these diseases were compiled via published research articles. The public databases viz chemspider, pubchem, pubmed were referred to incorporate the molecular weight, structure, IUPAC names of each plant molecule. In PENNDATABASE the search can be performed through diseases, plant molecules, CID or PMID. The collected data was stored using Mysql database. The commands to insert all the texts in the database were given by applying php-scripting language. Further, the web designing was carried out by html and css.

Figure 1A and 1B: The database with the physio- pathological and molecular details of the common neurodegenerative diseases



Design, Content and Utility of PENN database

The developed database contains the physio- pathological and molecular details of the common neurodegenerative diseases viz., Alzheimer's disease (AD), Amyotrophic lateral sclerosis (ALS), Parkinson's disease (PD), Huntington, and Creutzfeldt Jacob's (Figure 1A and 1B) and the chemical as well as plant derived drugs available for cure or prevention of these neurological diseases.

In the molecular basis section of the database, the link for gene and protein is given for retrieving sequence from NCBI and structures of target for each disease from PDB respectively. This is useful in performing sequence and structure comparison studies of the various target proteins. The database provides a comprehensive detail of the 51 different plant derived molecules known for their effectiveness in treatment of neurological disorders (Figure 2A and 2B). The CID and PMID provided in each plant derived natural molecules can be used for comparative studies on structure and pharmaco-properties of different plant molecules given in the database (Figure 3A, 3B and 3C).

The link to public databases such as NCBI, PDB, CID, Pubchem and KEGG is provided so as to increase the utility of the database and aid in new discoveries.

Acknowledgement

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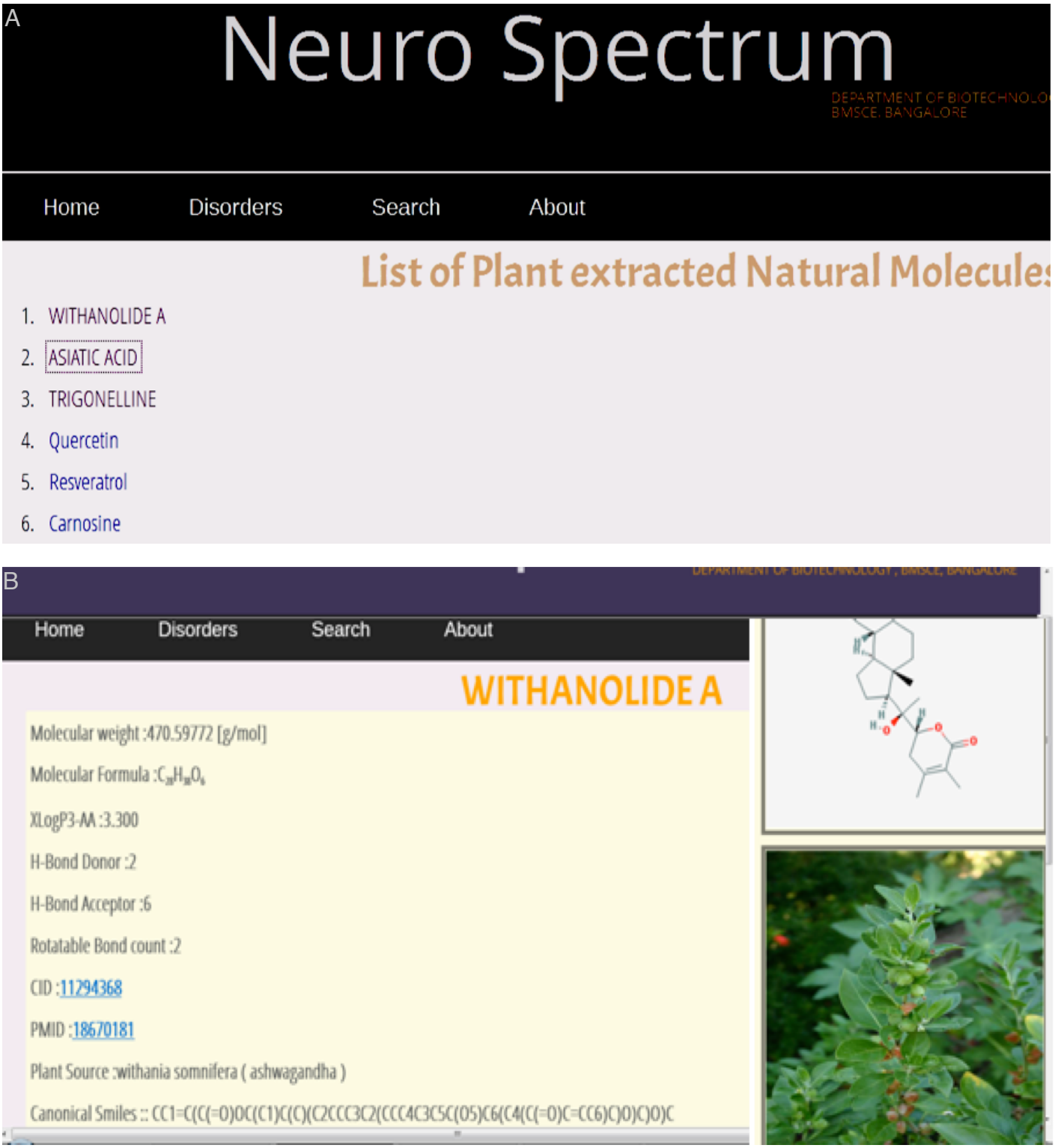
References

1. Trojanowski JQ, Arnold SE, Karlawish JH, Brunden K, Cary M, Davatzikos C, Detre J, Gaulton G, Grossman M, Hurtig H, et al.: **Design of comprehensive Alzheimer's disease centers to address unmet national needs**. *Alzheimer's & dementia : the journal of the Alzheimer's Association* 2010, **6**:150-155.
2. Rutkowski DT, Hegde RS: **Regulation of basal cellular physiology by the homeostatic unfolded protein response**. *The Journal of cell biology* 2010, **189**:783-794.
3. Hegde RS, Ploegh HL: **Quality and quantity control at the endoplasmic reticulum**. *Current opinion in cell biology* 2010,

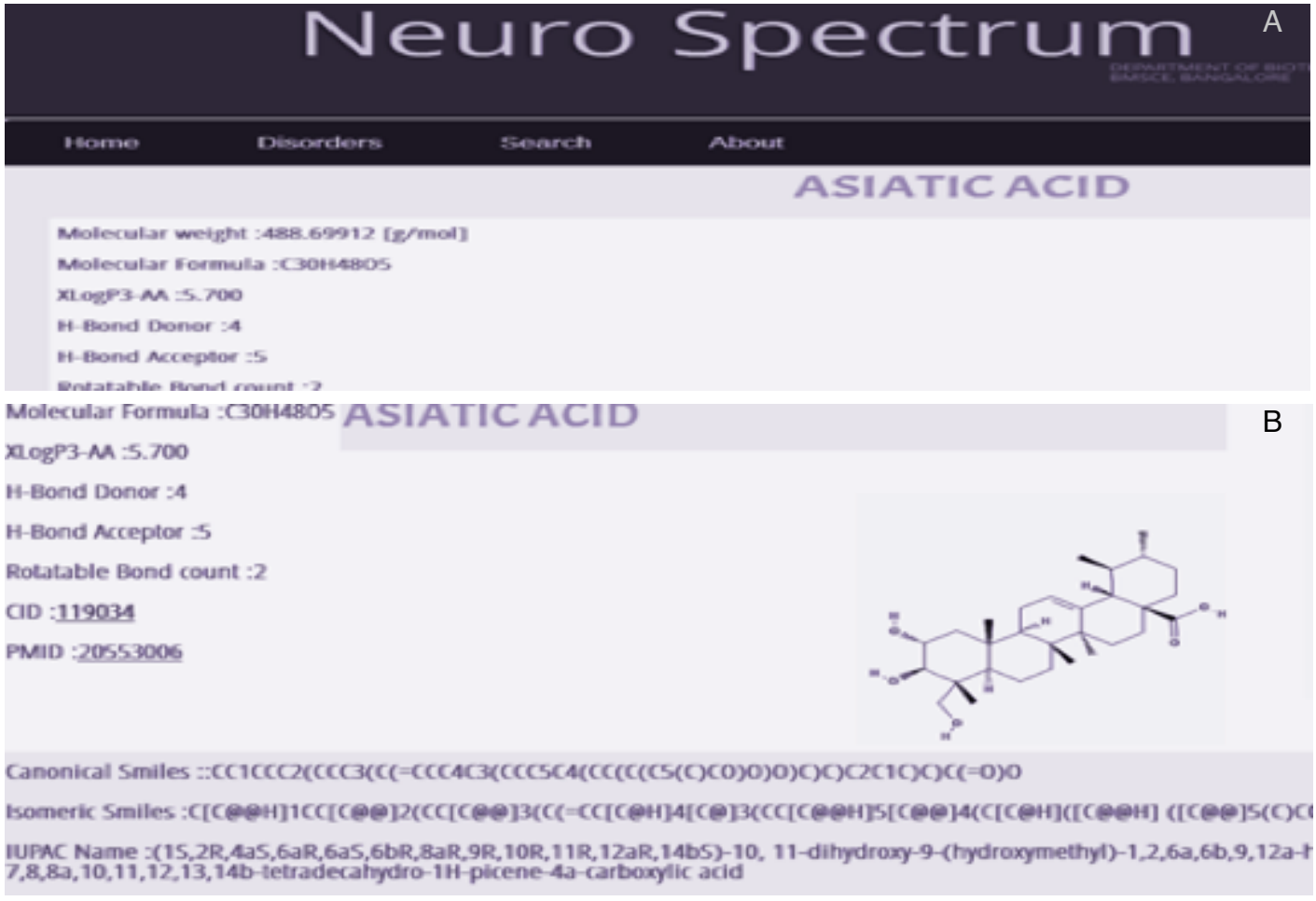
Fig.2A and 2B: The search section of database with 51 different plant derived natural molecules (2A) and biochemical, structural and source details of molecule (2B).



22:437-446.

4. Morimoto RI: **Proteotoxic stress and inducible chaperone networks in neurodegenerative disease and aging**. *Genes & development* 2008, **22**:1427-1438.
5. Chiti F, Dobson CM: **Protein misfolding, functional amyloid, and human disease**. *Annu. Rev. Biochem.* 2006, **75**:333-366.
6. Sutherland BA, Rahman R, Appleton I: **Mechanisms of action of green tea catechins, with a focus on ischemia-induced neurodegeneration**. *The Journal of nutritional biochemistry* 2006, **17**:291-306.
7. RajaSankar S, Manivasagam T, Sankar V, Prakash S, Muthusamy R, Krishnamurti A, Surendran S: **Withania somnifera root extract improves**

Figure 3A, 3B and 3C: The details of natural molecules as incorporated in database and link to CID and PMID to obtain detailed structure and pharmaco-properties of different plant molecules.



catecholamines and physiological abnormalities seen in a Parkinson's disease model mouse. *Journal of Ethnopharmacology* 2009, **125**:369-373.

8. Pyrzanowska J, Piechal A, Blecharz-Klin K, Lehner M, Skórzewska A, Turzyńska D, Sobolewska A, Plaznik A, Widy-Tyszkiewicz E: **The influence of the long-term administration of< i> Curcuma longa</i> extract on learning and spatial memory as well as the concentration of brain neurotransmitters and level of plasma corticosterone in aged rats**. *Pharmacology Biochemistry and Behavior* 2010, **95**:351-358.

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