



## Role of amino acids in genetic disorders and analysis of drugs based on Lipinski's rule

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### ABSTRACT

We have been demonstrating that the Distribution of Amino acids in Genetic Disorders. we retrieved that the diseased Proteome sequence for Genetic Disorders such as Anglemann Syndrome, Canavan disease, Celiac disease, Charcot Marie tooth Disease, Colour Blindness, Cridu chat, Cystic fibrosis, Down syndrome, Hemophilia and Neurofibrometasis. The Content of Polar amino acids are higher when compared with other type of amino acids. From the normal sequence, the Amino acids are mutated to Aspartic acid and Glutamic acid. If the amino acids are mutated to hydrophobic, hydrophilic and non polar amino acids we can control the genetic diseases. According to our work, based on Lipinski's rule we observed that Alverine, Ropinirole, Cyrimine, Carbidopa and Phosphatidylserine are the best controlling agent for Anglemann Syndrome, Canavan disease, Celiac disease, Charcot Marie tooth Disease, Colour Blindness respectively. We also observed that Mematine, Tyloxapol, Heaprin, Tranexamic acid and Indomethacin are the best drugs for Cridu chat, Cystic fibrosis, Down syndrome, Hemophilia and Neurofibrometasis respectively. Finally we concluded that, if the amino acids are mutated to hydrophobic or non polar amino acids, we can prevent Genetic Disorders.

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### Introduction

Depending on the polarity of the side chain, amino acids vary in their hydrophilic or hydrophobic character. These properties are important in protein structure and protein-protein interactions. The importance of the physical properties of the side chains comes from the influence this has on the amino acid residues' interactions with other structures, both within a single protein and between proteins.

The distribution of hydrophilic and hydrophobic amino acids determines the tertiary structure of the protein, and their physical location on the outside structure of the proteins influences their quaternary structure.

Hydrophilic and hydrophobic interactions of the proteins do not have to rely only on the side chains of amino acids themselves. By various posttranslational modifications other chains can be attached to the proteins, forming hydrophobic lipoproteins, or hydrophilic glycoproteins. The ratio of the polar and non-polar amino-acids seems to be a very important characteristic of the protein. [1]

#### Anglemann Syndrome

Angelman syndrome is a complex genetic disorder that affects the nervous system. Characteristic features of this condition include developmental delay or intellectual disability, severe speech impairment, seizures, small head size and problems with movement and balance. Delayed development can be noted by 6 months to 12 months of age, and other common signs and symptoms usually become apparent in early childhood. People with Angelman syndrome typically have a happy, excitable demeanor with frequent smiling and laughter, a short attention span, and hand-flapping movements. Some

affected individuals also have unusually fair skin and light-colored hair. [2]

#### Canavan Disease

Canavan disease is an autosomal recessive degenerative disorder that causes progressive damage to nerve cells in the brain. This disease is one of a group of genetic disorders called leukodystrophies.

Leukodystrophies are characterized by degeneration of myelin in the phospholipid layer insulating the axon of a neuron. The gene associated with the disorder is located on human chromosome 17. [3][4]

#### Celiac Disease

Celiac disease is a digestive disease that damages the small intestine and interferes with absorption of nutrients from food. People who have celiac disease cannot tolerate gluten, a protein in wheat, rye, and barley.

Gluten is found mainly in foods but may also be found in everyday products such as medicines, vitamins, and lip balms. When people with celiac disease eat foods or use products containing gluten, their immune system responds by damaging or destroying villi—the tiny, fingerlike protrusions lining the small intestine. [5]

#### Charcot-Marie-Tooth Disease (CMT)

Charcot-Marie-Tooth disease (CMT) is a heterogeneous inherited disorder of nerves that is characterized by loss of muscle tissue and touch sensation, predominantly in the feet and legs but also in the hands and arms in the advanced stages of disease. Presently incurable, this disease is one of the most common inherited neurological disorders, with 37 in 100,000 affected. [6][7]

### Cridu chat syndrome

Cri du chat syndrome, also known as chromosome 5p deletion syndrome, 5p minus syndrome or Lejeune's syndrome, is a rare genetic disorder due to a missing part of chromosome 5. [8]

### Colour blindness

Colour blindness is the inability to perceive differences between some of the colors that others can distinguish. It is most often of genetic nature, but may also occur because of eye, nerve, or brain damage, or due to exposure to certain chemicals. Color blindness is sometimes classed as a disability; in certain situations, however, color blind people have an advantage over people with normal color vision. There are some studies which conclude that color blind individuals are better at penetrating certain camouflages. [9]

### Cystic fibrosis

Cystic fibrosis is a genetic disorder known to be an inherited disease of the secretory glands, including the glands that make mucus and sweat. The hallmarks of cystic fibrosis are salty tasting skin, normal appetite but poor growth and poor weight gain, excess mucus production, and coughing/shortness of breath. Males can be infertile due to the condition congenital bilateral absence of the vas deferens. Often, symptoms of CF appear in infancy and childhood. Meconium ileus is a typical finding in newborn babies with CF. Although technically a rare disease, cystic fibrosis is ranked as one of the most widespread life-shortening genetic diseases. It is most common among nations in the Western world; one in twenty-two people of Mediterranean descent is a carrier of one gene for CF, making it the most common genetic disease in these population. [10] [11]

### Down syndrome

Down syndrome (DS), also called Trisomy 21, is a condition in which extra genetic material causes delays in the way a child develops, both mentally and physically. It affects about 1 in every 800 babies. The physical features and medical problems associated with Down syndrome can vary widely from child to child. [12][13] [14]

### Hemophilia

Hemophilia is a disease that prevents blood from clotting properly, so a person who has it bleeds more than someone without hemophilia does. It's a genetic disorder, which means it's the result of a change in genes that was either inherited or occurred during development in the womb. Sticky cells in the blood called platelets go to where the bleeding is and plug up the hole. This is the first step in the clotting process. When the platelets plug the hole, they release chemicals that attract more sticky platelets and also activate various proteins in the blood known as clotting factors. [15] [16]

### Neurofibromatosis

Neurofibromatosis is autosomal dominant, which means that it affects males and females equally and is dominant. Therefore, if only one parent has neurofibromatosis, his or her children have a 50% chance of developing the condition as well. Disease severity in affected individuals, however, can vary. Moreover, in around half of cases there is no other affected family member because a new mutation has occurred. [17]

### Methodology

❖ Retrieved the Genetic Disorders protein sequences from NCBI.

❖ The sequences were saved in notepad and submitted in to C Program.

❖ Amino acid compositions for all the disorder sequences are calculated using C program.

❖ The values are stored in the MS-Excel and Graph drawn for all types of amino acids and Genetic disorders.

❖ The list of drugs were retrieved from drug bank for each Genetic Disorders

❖ Based on Lipinski's rule the parameters are calculated like Hbond donor, Hbond acceptor, Log P and Molecular weight.

❖ Hbond donors, Hbond acceptors and Mol.wt were calculated by Pubchem compound database and Log P values calculated by ALOGPS tool.

❖ Finally all the results are compared and discussed.

### Lipinski's rule-of-five analysis

Christopher Lipinski's rule-of-five analysis helped to raise awareness about properties and structural features that make molecules more or less drug-like. The guidelines were quickly adopted by the pharmaceutical industry as it helped apply ADME considerations early in preclinical development and could help avoid costly late-stage preclinical and clinical failures. The guidelines predict that poor absorption or permeation of a orally administered compound are more likely if the compound meets the following criteria:

The Rule of 5" got its name from the cutoff values for each of the four parameters that define the "drug-likeness" of the potential drug candidates: all of these values are close to five or a multiple of five. In the USAN set we found that the sum of Ns and Os in the molecular formula was greater than 10 in 12% of the compounds. Eleven percent of compounds had a MWT of over 500. Ten percent of compounds had a CLogP larger than 5 (or an MLogP larger than 4.15) and in 8% of compounds the sum of OHs and NHs in the chemical structure was larger than 5. The "rule of 5" states that: poor absorption or permeation is more likely when:

- There are more than 5 H-bond donors
- The MWT is over 500
- The Log P is over 5
- There are more than 10 H-bond acceptors

Tab 1: Distribution of Amino acids In Genetic Disorders

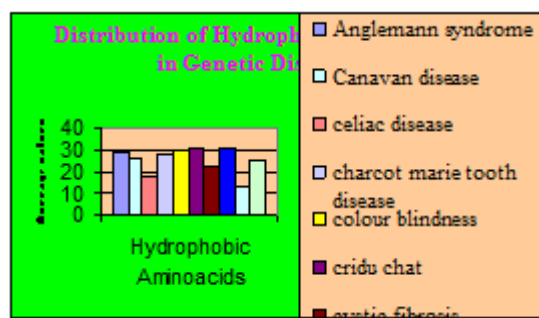
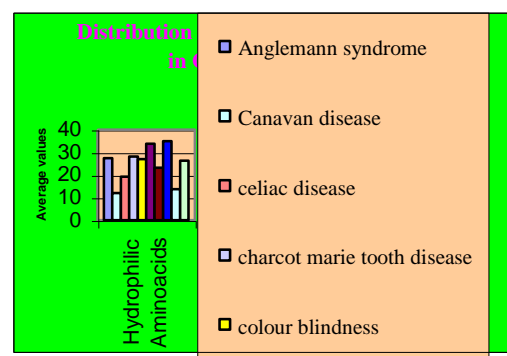
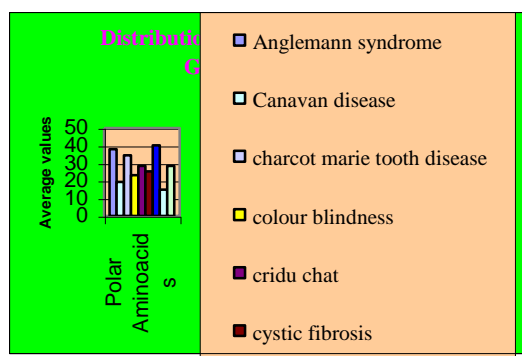
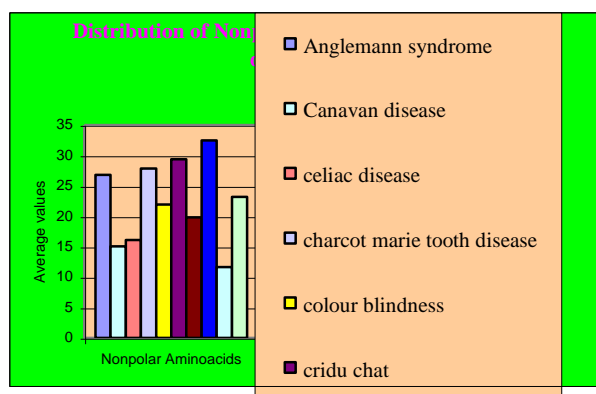


Fig 1: Distribution of Hydrophobic amino acids in Genetic Disorders



**Fig 2: Distribution of Hydrophilic amino acids in Genetic Disorders****Fig 3: Distribution of Polar amino acids in Genetic Disorders****Fig 4: Distribution of Nonpolar amino acids in Genetic Disorders**

## Discussion

Table 1 shows that the Distribution of Hydrophobic, Hydrophilic, Polar and Non-polar Amino acids in Genetic Disorders such as Anglemann syndrome, Canavan disease, Celiac Disease, Charcot Marie Tooth disease, Colour Blindness, Cridu chat Syndrome, Cystic Fibrosis, Down Syndrome, Hemophilia and Neurofibrometasis.

In Anglemann syndrome, distribution of Polar amino acids (Aspartic acid and Glutamic acid) are highly present (Fig 1). So, it may cause the syndrome. Hydrophobic and Hydrophilic amino acids content are lower than the polar amino acids in Anglemann Syndrome. In Canavan Disease, Hydrophobic amino acids are highly present where as Hydrophilic, Polar and Non-polar amino acids are very less (Fig 2).

Fig 3 shows that Polar amino acids composition is high when compared with other amino acids in Celiac Disease. In Charcot Marie Tooth Disease, the content of Polar amino acids is high ( Fig 4). From the normal sequence, the amino acids are mutated to Polar amino acids. In Colour Blindness, even hydrophobic amino acids content is high, the hydrophilic, polar and non-polar amino acids are mutated and it may cause Color Blindness (Fig 5).

In Cridu Chat Syndrome, the residues are mutated to Hydrophilic and Hydrophobic amino acids(Fig 6). So it causes this syndrome. Fig 7 shows that the content of Polar amino acids are higher than Hydrophobic and Hydrophilic residues in Cystic Fibrosis. The Distribution of Non polar amino acids are very low. Due to this reason, Cystic Fibrosis may be caused.

In Down syndrome from the normal sequence the amino acids are mutated to Polar amino acids (Fig 8). So, only it causes the syndrome. Fig 9 shows s that the distribution of Polar amino acids is high when compared with other amino acids.

Neurofibrometasis also have the high content of Polar amino acids (Fig 10). So, it may cause the disease.

Fig 11 shows that the distribution of hydrophobic aminoacids in genetic disorders. Hydrophobic residues are highly contributed in Colour blindness. Fig 12 shows that the distribution of hydrophilic amino acids in genetic disorders. Hydrophilic residues are highly present in Down syndrome.

Fig 13 shows that the distribution of polar aminoacids in genetic disorders. Polar aminoacids are highly present in disorders.Fig 14 shows that the distribution of non polar aminoacids in genetic disorders.Very low content of non-polar aminoacids iare present in disorders.

In all Genetic Disorders, Hydrophobic, Hydrophilic and Non Polar amino acids are very low when compared with Polar amino acids. The mutation, which converts from Non-polar amino acids to Polar, Hydrophobic and Hydrophilic Residues. If non-polar amino acids cannot mutate to other amino acids, we may control the Genetic Disorders.

The drugs retrieved for all genetic disorders from drug bank and analyzed the best drug based on Lipinski's Rule. Hbond donors, Hbond acceptors and Mol.wt are calculated by Pubchem compound database and Log P values are calculated by ALOGPS tool. Table 2-11 shows that the calculation of drug parameters for Anglemann syndrome, Canavan disease, Celiac Disease, Charcot Marie Tooth disease, Colour Blindness, Cridu chat Syndrome, Cystic Fibrosis, Down Syndrome, Hemophilia and Neurofibrometasis respectively.

Based on Lipinski's rule and Absorption of the drugs, I analyzed that the best curing agents for each genetic disorder. Table 12-21 shows that absorption of the drugs for Anglemann syndrome, Canavan disease, Celiac Disease, Charcot Marie Tooth disease, Colour Blindness, Cridu chat Syndrome, Cystic Fibrosis, Down Syndrome, Hemophilia and Neurofibrometasis respectively. Absorption is very essential for Distribution, Metabolism, Excretion and Toxicology.

## Conclusion

I have observed that the results for Genetic Disorders, which includes the distribution of amino acids and absorption analysis of the drugs.

When compare with Hydrophobic, Hydrophilic and Non-polar amino acids, the polar amino acids are highly present in all genetic disorders. From the normal sequence, the amino acids are mutated to Aspartic acid and Glutamic acid. Due to the above reason, genetic disorders may be caused. If the amino acids are mutated to Hydrophobic, Hydrophilic or non-polar amino acids, we can reduce the risks of genetic disorders. If we increase the non-polar amino acids, we may control the genetic disorders.

According to my project, based on Lipinski's rule, I have observed that Alverine, Ropinirole, Cycrimine, Carbidopa and Phosphatidyl serine are the best curing agents for Anglemann syndrome, Canavan disease, Celiac disease, Charcot Marie Tooth disease and Colour blindness respectively.

I also observed that Memantine, Tyloxapol, Heparin, Tranexamic acid and Indomethacin are the best curing agents for Cridu chat syndrome, Cystic fibrosis, Down Syndrome, Hemophilia and Neurofibrometasis respectively.

Finally, I concluded that, if the amino acids are mutated to hydrophobic or non-polar amino acids, we could prevent the genetic disorders. These drugs which satisfy the Lipinski's rule and it has a good absorption capacity when compared with other drugs. Absorption is very essential for Distribution, Metabolism,

Excretion and Toxicology.

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### Aminoacids results

#### Distribution of aminoacids in genetic disorders

Genetic disorder	Hydrophobic aminoacids	Hydrophilic aminoacids	Polar aminoacids	Nonpolar Aminoacids
Anglemann syndrome	29.02857	27.45143	37.985715	26.828573
Canavan disease	26.426668	11.986665	19.333335	15.044443
Celaic disease	17.872518	19.16641	20.801525	16.091603
Charcot marie tooth disease	27.952632	28.067368	34.46842	27.856143
Colour blindness	29.899998	26.999996	23.222225	21.92592
Cridu chat	31.136842	33.757896	28.421055	29.385966
Cystic fibrosis	23.14121	23.139482	25.44092	19.818443
Down syndrome	30.729187	34.856344	40.22462	32.503386
Hemophilia	12.523404	13.778723	14.898935	11.670212
Neurofibrometasis	25.725233	26.298134	28.422895	23.169783

## Drugs results

## Results for anglemann syndrome

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Alverine	1	1	5.56	317.896
Tegaserod	4	6	1.03	301.386
Methadone	0	2	3.9	309.445
Alosetron	2	5	0.60	243.264
Thiopropazine	0	0	3.09	446.629

Tab 2: Calculation of Drug Parameters for Anglemann Syndrome

## Results for canavan disease

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Olsalazine	4	8	1.13	302.239
Penicillamine	2	3	-1.70	149.211
Ropinirole	1	2	3.16	260.374
Entacapone	2	6	2.50	305.286
Mesalazine	2	4	0.15	152.127

Tab 3: Calculation of Drug Parameters for Canavan Disease

## Results for celiac disease

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Prednisolone	3	5	1.66	360.444
Seligiline	0	2	3.08	186.285
Cycrimine	1	4	4.15	287.439
Pramipexole	2	3	2.18	211.327

Tab 4: Calculation of Drug Parameters for Celiac Disease

## Results for charcot marie tooth disease

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Carbidopa	5	6	-0.16	226.229
Clopidorel	0	3	3.84	327.777
Enprofylline	2	3	3.03	194.190
Amlexanox	2	6	3.10	298.293
Phentolamine	2	4	2.60	281.352

Tab 5: Calculation of Drug Parameters for Charcot Marie Tooth Disease

## Results for colour blindness

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Butylamine	1	1	0.85	73.13684
Tazarotene	0	3	5.15	351.4619
Vitamin A	1	1	6.38	286.4516
Phosphatidylserine	3	11	-1.02	385.3041

Tab 6: Calculation of Drug Parameters for Colour Blindness

## Results for cridu chat

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Glycerol	3	3	-1.93	92.09382
Mematine	1	1	3.31	179.3018

Tab 7: Calculation of Drug Parameters for Cridu Chat Syndrome

## Results for cystic fibrosis

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
DornaseAlfa	0	5	3.70	216.5357
Pancrelipase	0	6	1.35	329.4640
Tyloxapol	1	3	5.50	280.4024
Sulfinpyrazone	0	3	2.92	404.4815
Fenfluramine	1	4	3.30	231.2573

Tab 8: Calculation of Drug Parameters for Cystic Fibrosis

## Results for down syndrome

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Heparin	15	38	-10.8	1134.9278
Aspartame	3	6	-1.18	294.30312
Nandralone	1	2	2.60	274.39784
Trilostane	1	4	2.80	329.43328
Desipramine	1	2	4.02	296.50231

**Tab 9: Calculation of Drug Parameters for Down Syndrome  
Results for hemophilia**

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Tranexamicacid	2	3	-1.42	157.2102

**Tab 10: Calculation of Drug Parameters for Hemophilia  
Results for neurofibrometasis**

DRUGS	Hbond Donar	Hbond Acceptor	Log P	Mol.wt
Indomethacin	1	4	5.25	357.7876

**Tab 11: Calculation of Drug Parameters for Neurofibrometasis  
Absorption results**

**Absorption analysis for anglemann syndrome**

DRUGS	A	B	C	D	Absorption
Alverine	0	0	1	0	Good
Tegaserod	0	0	0	0	Poor
Methadone	0	0	0	0	Poor
Alosetron	0	0	0	0	Poor
Thiopropazine	0	0	0	0	Poor

**Tab 12: Absorption Analysis of the drugs for Anglemann Syndrome**

**Absorption analysis for canavan disease**

DRUGS	A	B	C	D	Absorption
Olsalazine	0	0	0	0	Poor
Penicillamine	0	0	0	0	Poor
Ropinirole	0	0	1	0	Good
Entacapone	0	0	0	0	Poor
Mesalazine	0	0	0	0	Poor

**Tab 13: Absorption Analysis of the drugs for Canavan Disease**

**Absorption analysis for celaic disease**

DRUGS	A	B	C	D	Absorption
Prednisolone	0	0	0	0	Poor
Seligiline	0	0	0	0	Poor
Cycrimine	0	0	1	0	Good
Pramipexole	0	0	0	0	Poor

**Tab 14: Absorption Analysis of the drugs for Celiac Disease**

**Absorption analysis for charcot marie tooth disease**

DRUGS	A	B	C	D	Absorption
Carbidopa	0	0	0	0	Poor
Clopidorel	0	0	1	0	Good
Enprofylline	0	0	0	0	Poor
Amlexanox	0	0	0	0	Poor
Phentolamine	0	0	0	0	Poor

**Tab 15: Absorption Analysis of the drugs for Charcot Marie Tooth Disease**

**Absorption analysis for colour blindness**

DRUGS	A	B	C	D	Absorption
Butylamine	0	0	0	0	Poor
Tazarotene	0	0	0	0	Poor
Vitamin A	0	0	0	0	Poor
Phosphatidylserine	0	1	0	0	Good

**Tab 16: Absorption Analysis of the drugs for Colour Blindness**

**Absorption analysis for cridu chat syndrome**

DRUGS	A	B	C	D	Absorption
Glycerol	0	0	0	0	Poor
Mematine	0	0	1	0	Good

**Tab 17: Absorption Analysis of the drugs for Cridu Chat Syndrome****Absorption analysis for cystic fibrosis**

DRUGS	A	B	C	D	Absorption
DornaseAlfa	0	0	0	0	Poor
Pancrelipase	0	0	0	0	Poor
Tyloxapol	0	0	1	0	Good
Sulfinpyrazone	0	0	0	0	Poor
Fenfluramine	0	0	0	0	Poor

**Tab 18: Absorption Analysis of the drugs for Cystic Fibrosis****Absorption Analysis for Down Syndrome**

DRUGS	A	B	C	D	Absorption
Heparin	1	1	0	1	High
Aspartame	0	0	0	0	Poor
Nandralone	0	0	0	0	Poor
Trilostane	0	0	0	0	Poor
Desipramine	0	0	0	0	Poor

**Tab 19: Absorption Analysis of the drugs for Down syndrome****Absorption analysis for Hemophilia**

DRUGS	A	B	C	D	Absorption
Tranexamic acid	0	0	0	0	Poor

**Tab 20: Absorption Analysis of the drugs for Hemophilia****Absorption analysis for neurofibrometasis**

DRUGS	A	B	C	D	Absorption
Indomethacin	0	0	1	0	Good