August 20, 2024

* Choosing a topic:

- Some things that intrigue me are researching, ayurveda, psychology of rapist (How/what they think), How are video games able to allure teens (sensations, etc),

- I think all these topics are great but I want to do a research project on Ayurveda* since not a lot of research has been done in this are I think it'll be interesting to "dig up things".

* How can we integrate ayurveda in modern medication to better the quality of treatment for patients

August 20, 2024

* Starting Background Research.

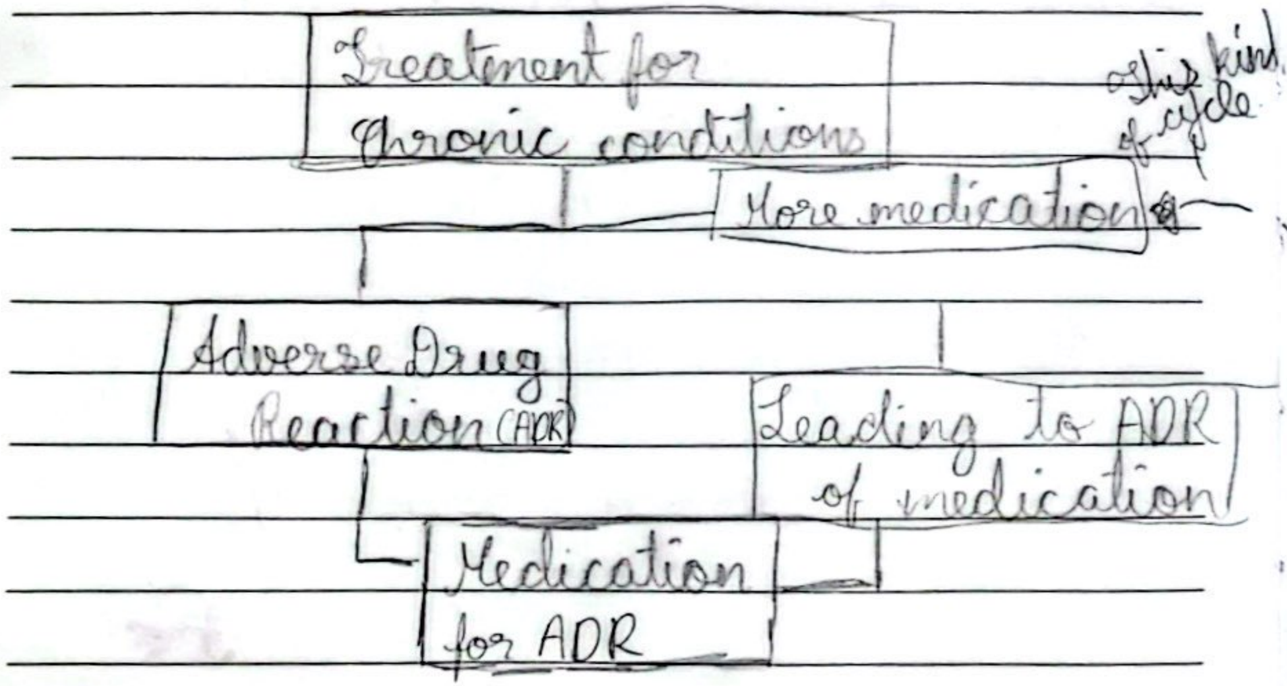
- Adverse Drug Reaction (ADR): International conference on harmonisation of Technical Requirements for registration of Pharmaceuticals for Human Use, which (WHO and FDA are part of) defines ADR as "response to a drug which is unintended and occurs at doses normally used for treatment of a desease"

- ADR are a serious problem: In 2022, there were over 1.25 million adverse events reported and nearly 175 000 death. Thus, ADRs increase morbidity, mortality, hospitalizations, and healthcare costs, efforts to prevent their occurence must be prioritized.

- Link: ncbi.nlm.nih.gov/books/NBK599521/

• Chronic desease treatments:

- As the prevalence of chronic conditions is growing, the treatment of these conditions is leading to a poor quality of life for the patients because chronic desease treatment have side effects, medication for these side effects have their own side affects and the cycle continues...



• Sp

* Specific reasons why the side effects of chronic desease treatments should not be treated with conventiontion medicines and how treating the side effects of chronic desease treatments leads to a poor quality of life for patients.

① Increased Risk of more side effects:
- Using conventional medication to manage side effects of chronic disease treatment leads ~~to forming a cycle to~~ to a need for more medication to manage the side effects of the medication already being used to manage the side effects of chronic desease treatment, forming a cycle. Since each medication can have its own side effects.

② Overmedication: Relying on multiple medications to ~~cont~~ counter the side effects of chronic desease treatments can lead to overmedication, causing

additional health problems like dependence on certain drugs, reduced cognitive function, and even organ damage over time.

* Polypharmacy: Use of more five medication or the use of at least one potentially inappropriate drug, continues to rise. Polypharmacy typically occurs after chronic disease treatment, in order to manage side effects

August 23, 2024

Continued...

③ Masking Underlying Issues:
- Medications treating side effect of chronic disease treatments mask underlying issues without addressing the root cause of the problem, leading to a lack of focus on lifestyle changes or alternative therapies that are beneficial in the long-term. So, essentially ~~[illegible]~~ conventional medications hides the problem without actually resolving it.

④ Psychological Impact:
- For patients, constantly dealing with side effects and the need for additional medications can be psychologically draining, leading to feelings of frustration, ~~helpless~~ helplessness, or anxiety

* Healthcare providers must consider non-pharmacological approaches, lifestyle changes, or alternative therapies to manage side effects of chronic disease treatments to manage them effectively and minimizing the risks associated with taking multiple medication. Overall improving the overall quality of treatment and its outcomes for the patients.

Link: Report: Seniors and the healthcare system: What is the impact of multiple Chronic Conditions

August 25, 2024

- Ayurveda: Traditional Indian system of medicine, almost 4000 years old

- Ayurveda treatments focus on addressing the root cause of a problem and the overall health of a problem.

- Ayurveda uses nutrition, lifestyle changes, and natural treatments.

- It isn't well-researched yet, but in countries like India it's practiced in the same way ~~as~~ that standard medicine is used in U.S.

Link: Ayurveda: John Hopkins medicine

August 26, 2024

- Ayurvedic treatments generally have minimal to no side effects since ayurveda herbs comprise of fruits, spices, vegetables and natural herbs

- Moreover, even the minimal side-effects can be avoided by taking herbs in quantities recommended by a proffetional

- A key principal of ayurveda is individualism, and every ayurveda treatment recommended by a practitioner is based on individual needs of a patients considering all medications that they are already taking and any allergies that they might have, reducing the risk of allergic reaction and intervention with medicine.

- The only other con is heavy metals found in herbs because they are either grown on contaminated soil or heavy metals are used in the processing of these herb. This risk can be avoided by purchasing organic vegetables and pills from brands recomended by an ayurveda practitioner.

Link: MM Department of Health: Metal toxicity from Ayurvedic Medication

Ayurveda institute in Kerala: Health Benifits of Ayurveda Over modern medicine

August 27, 2024

- For my project, I plan to compare Ayurveda and modern medicine in treating the side effects of treatment for chronic diseases through bioinfomatrics.

- Bioinfomatrics: Using computer data to collect, store and analyze Biological data

- Bioinfomatrics can be really helpful and essential in completing my project because I can collect, store, and analyze data to compare Ayurveda medicine v.s conventional medicine in terms of compound properties, Molecular docking scores / Binding affinity scores, Log P values, P-values, Fold changes, LD50 values, Toxicity classes, and probability scores.

August 28, 2024

- After looking at some papers on Google Scholar I have come up with a rough methodology for my research paper

① Make a list of the common chronic diseases and their treatment options

② Make another list of the common side effects of treatment.

③ Finally, make a list of Ayurveda herbs used to treat the side effects

④ Make another list of conventional medication used to treat the side-effects

* I am doing a component-based approach for my research, where my focus is on analyzing the bioactive compounds within the herbs.

August 28, 2024

⑤ Gather info about the bioactive compounds found in Ayurveda herbs selected

* My research will focus primarily on safety & toxicity comparison, as well as the efficacy comparison between Ayurveda and conventional medicine.

⑥ Predict target proteins: Which proteins or genes are involved in the side effects

⑦ ligand preparation: Once the bioactive compounds are identified, their 3D structure (ligands) are obtained, this is important for our next step docking.
- For most compounds, 3D structures are accesible on databases like PUBChem, ChEbI, and ZINC. But if only 2D models, generate 3D models using molecular modelling software like ChemSketch, OpenBabel, and Avogadro, AutodockTools.

* How to identify bioactive compounds in Ayurveda herbs.

- Literature Review: Some "popular" herbs have been studied extensively and the bioactive compounds may be documented.

- There are also databases to identify compounds
- Dr. Duke's Phytochemical and Ethnobotanical Databases.
- TCMSP (Traditional Chinese Medicine Systems Pharmacology Database.

(P.S. Bioactive Compounds: A type of chemical found in plants and certain foods, affecting directly affecting a living organism)

* - Minimize Energy: Ensures that the ligand structure is in its lowest energy conformation making it biologically relevant, and removing unrealistic bond length / angles. Use programs like Avogadro, Openbabel, or molecular dynamic packages like GROMACS and AMBER these relax the structure by applying forces.

- Assign Charges: Proper atomic charges must be assigned to ligand, because electrostatic interactions (forces between nearby atoms and molecules) between the ligand and the target protein play a critical role in accuracy of results.
- AutoDock Tools can assign Gasteiger charges.

* This is a lot of words so a quick summary of step 7:

① Download the ligand from PubChem
② Open in Avogadro, add hydrogen, minimize energy
③ Convert the structure to PDBQT format and assign Gasteiger charges using AutoDockTools
④ Save the ligand in the appropriate format.

- The same steps applies to finding the ligand on conventional drugs, just use the chemicals used in drugs, not bioactive compounds

August 30, 2024

⑧ Molecular Docking Scores: Predict how well a ligand binds to a target protein/enzyme, how it interacts with the target protein/receptor/enzyme involved in the side effect. In comparing modern and and ayurveda medicine, docking scores help determine the potential efficacy of a compound.
- Can be performed using tools like AutoDock, PyMOL, and Schrondinger, that stimulate drug and target protein interaction, calculating binding affinity between the compound and the target, represented by a docking score (lower score = stronger binding = higher efficacy)

⑨ Log P values: Indicate the lipophilicity (how fat soluble), how easily a compound crosses cell membranes, which is important for absorption and distribution of the herb/drug. An oral drug/herb should

have a LOGP ~~value~~ value. of <5. Use swiss ADME to calculate LOGP value

* Oral drug: taking medication through mouth.

⑩ LD50 (Lethal dose 50%): Dose of substance that kills 50% of a test population and is used to estimate a drug's toxicity (lower LD50 value = higher toxicity = more dangerous treatment). LD50 values help assess the safety of modern v.s ayurveda medicine, if ayurveda has a lower LD50 value than a synthetic drug, it could be prefferred, despite possibly lower efficacy, for long term usage
- Typically determined through experiments where different doses of a drug are administered, and the dose that kills half the subjects is recorded as the LD50 value. But for the sake of this research, I will use tools like Pro Tox-II and pKCSM to predict the compounds LD50, and also the toxicity classes.

⑪ Toxicity Classes (Optional step only if time left): ProTox-II and pkCSM classify compounds into toxicity classes ranging from safe (class V) to highly toxic (class I). Toxic classes are categories that define the severity of a substance's toxic effects, based on data like LD50 value, exposure routes, and specific effects. Comparing toxicity classes helps determine treatments (modern v.s ayurveda) are safer for patients, acting as a comprehensive risk assesment). If a herb has fewer toxic effects than a synthetic drug, it could be proffered, despite possibly lower efficacy, in the longer term use.

- For each Target Protein, explain why I chose it, like the specific link between Protein and side effect.

- For each herb explain why I chose it, like the roles of the bioactive compounds in resolving the side effect.

Sept. 5, 2024

Log P value

Lipinski's Rule of 5

Introduced by Pfizer's Lipinski in 1997. Determines drug

Called rule of 5 because number are multiples of 5

- Lipinski's rule of 5: Guideline used in drug discovery and development to evaluate drug-like entities and determine their potential as oral drug candidates in humans.

- The rule states that a compound is more likely to have poor absorption or permeation if it violates any of the following conditions:

① Molecular weight over 500 g/mol
② More than 5 hydrogen bond donors
③ More than 10 hydrogen bond acceptors
④ A calculated log P value over 5.

- The rule is commonly used to assess oral bioavailability of drug molecules and has been influential in preclinical drug development.

- Oral bioavailability: The fraction (%) of an administered drug that reaches the systemic circulation (blood)

- To determine the exact bioavailability (a percentage), experimental studies in animals or humans are required.

- Bioavailable: The ability of a drug or other substance to be absorbed and used by the body. Is measured on a continuous range from 0-1.

- Bioavailability

Absolute Bioavailability	Relative bioavailability:
Bioavailability of an orally administered drug is compared with the bioavailability obtained of the same drug when it is administered intravenously. Measures how much of a drug administered via a non-intravenous route (e.g. oral, inhal-	Bioavailability of a formulation of a certain drug (A) is compared with another formulation (B) of the same drug. E.g. Comparing the bioavailability of a tablet versus a liquid form of the same drug

systemic circulation (blood) compared to the same drug given intravenously e.g. If a drug has 50% absolute bioavailability, only half of the dose given orally reaches into the bloodstream.

2 core categories of bioavalability

- Since the purpose of this research is to propose Ayurvedic herbs as an alternative of oral drugs taken to manage side effects of chronic disease treatments, it is important to see how well these herbs can be absorbed when taken orally, because it doesn't matter how well a compound binds with a target protein if the body isn't able to absorb it

- That is knowing the absolute bioavailability is extremely important

Sept. 6, 2024

* Absolute Bioavailability Ratings:

- High (>85%):
Indicates that a large proportion of drug doses reaches systemic circulation (blood). Considered very efficient

- Moderate (50% - 85%):
Indicates decent absorption.

- Low (<50%)
Indicates poor absorption, may require higher doses or alternative intravasive methods (eg. injections).

* Absolute Bioavailability formula:

$$F_{abs} = \left(\frac{AUC_{non\,IV} \times Dose_{IV}}{AUC_{IV} \times Dose_{non\,IV}} \right) \times 100$$

Where:

$AUC_{non\text{-}IV}$: The area under the concentration-time curve (AUC) for the non-IV route

AUC_{IV}: The area under the concentration-time curve (AUC) for the IV route

$Dose_{non\text{-}IV}$: The dose administered via the non-IV route.

$Dose_{IV}$: The dose administered via the IV route

AUC - Sept. 9, 2024

- Area Under the Curve (AUC): Reflects exposure to a drug after administration, how much drug reaches a persons bloodstream in a given period of time after a dose is given.

- The "curve" refers to a graph of drug concentration (amount in the blood) on the

y-axis verses time on the x-axis

- When you take a drug, its concentration in the blood starts low, increasg as it's absorbed, peaks, and then decreases as your body breaks it down and eliminates it, creating a curve AUC is the total area under this curve, representing the total drug exposure your body has experienced

Why is AUC important:

Drug absorption: Tells us how much of the drug actually entered the bloodstream

Drug effectiveness: More exposure (higher AUC) means the drug has a better chance to work

Methods to get AUC

What we'll need:

- Drug concentration measurements taken at different time points.

- Our blood is primarily composed of red blood cells (carriers of nutrients and oxygen) + plasma (liquid portion of blood, where red and white cells float) .. + white blood blood cells

When measuring the drug concentration, a sample of whole blood is draw from the patient, then the red blood cells, white blood cells, and plasma are seperated. The plasma is withdrawn and analyzed for drug concentration and red + white cells are discarded.

$Amount_{blood} = Amount_{WBC} + Amount_{RBC}$

- Measurement from when the drug was first administered, until the drug concentration becomes negligible (essentially 0)

* AUC is just raw data which tells us how much drug concentration there was in the body, but absolute bioavailability helps

us quantify the data, by comparing oral to IV, since IV will have the highest AUC and bioavailability, comparing oral AUC to it gives us an idea of the potential of the drug orally. So if the absolute bioavailability is 750% then we know the drug is effective but if it's less than 50% than we know that administering the drug through IV would be a better choice or finding ways to improve it's bioavailability. AUC played a big role in reaching this conclusion, because raw data (AUC) has to analyzed C absolute bioavailability in order to come to an observation.

- It would been really beneficial, to have experimented and determined the AUC and absolute bioavailability, in determining the efficiency and absorption of overseeding herbs, but unfortunately since it require me to do blood related experiments on humans (animals and also due to the lack of resources & am unable to conduct experiments regarding AUC and absolute bioavailability

- The most versatile and commonly used approach for calculating the AUC is the linear Trapezoidal Method. This method is the standard and required by OGD and FDA. The linear trapezoidal method uses linear interpolation between data points to calculate AUC.

- Linear interpolation: If the two known points are given by the coordinates (x_0, y_0) and (x_1, y_1) the linear interpolant is the straight line between these points
Calculates the area under this line segment as a trapezoid

Formula:

$$AUC = \frac{1}{2}(C_1 + C_2)(t_2 - t_1)$$

Where:

C_1 and C_2 : Drug concentrations at times t_1 and t_2.

$t_2 - t_1$: Time interval between the two data points.

Concept:

- The first term, $\frac{1}{2}(C_1 + C_2)$, calculates the average drug concentration over the time interval.
- The second term, $(t_2 - t_1)$, represents the duration of that interval.
- Multiplying these gives the area under the curve for that segment.

Summation:

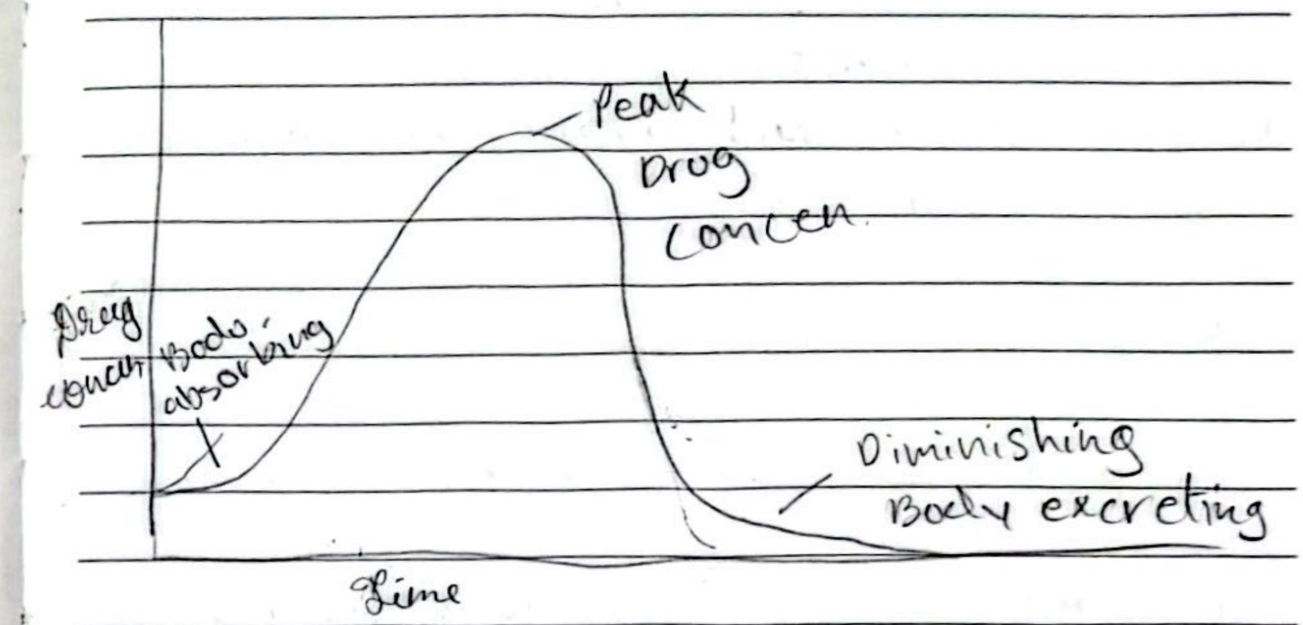
- Add the AUCs of all time intervals to get the total AUC:

Total AUC = sum of AUC of all time intervals

Average drug concentration over the total time interval:

$$C_{avg} = \frac{\text{Total AUC}}{\text{Total time}}$$

AUC diagram:



- Unfortunately, as we discussed earlier, we can't use AUC and absolute bioavailability to determine the oral bioavailability of ayurveda herbs. So we can use Lipinski's rule of 5, a reliable and widely used method to predict the oral bioavailability of ayurveda herbs.

4 components of Lipinski's rule of 5:

should not be
① Molecular weight over 500 g/mol:
- Molecular size affects absorption. Because larger molecules likely contain more polar functional groups, so in principle are less readily absorbed through cell membranes

- Polar functional groups are parts of a molecule with an uneven distribution of electric charges due to differences in electronegativity between atoms. This makes them water-attracting (hydrophillic)

- Electronegativity: A chemical property that describes the tendency of an atom to attract electrons towards itself

there usually more
- In large molecules, polar functional groups' ~~[illegible]~~, meaning there are more polar regions on the molecule, which favor interactions with water, than non polar regions, which favor interactions with lipid (fat) environments. This domination of polar funtional groups, leads to favoring interactions with water, increasing the molecules hydrophilicity.

- In small molecules, polar funtional groups have less influence, due to extensive non-polar (hydrophobic) regions, have large non-polar regions. This results in increased lipophilicity and decreased water solubility, favoring interactions with lipid environments.

- Lipophilicity: Refers to a molecule's affinity for lipids or fat-like environment (e.g. cell membrane) Dissolve in lipids.

- Hydrophilicity: Affinity to water

- Hydrophobicity: Refers to a molecule's tendency to avoid water or aqueous environments. A molecule is hydrophobic if it has few or no polar groups.

- Highly Polar Drugs = Hydrophilic Drugs = large: Dissolve well in aqueous environments, like the gastrointestinal (GI) tract, because of their high water solubility. However, their absorption across cell membranes (which have a lipid bilayer) is limited because they cannot easily easily diffuse through the lipophilic membrane.

- Non polar Drugs = lipophilic drug = small lipophilicity generally enhances membrane permeability, aiding in absorption. Lipophilic drugs pass easily through the lipid bilayer of cell membranes. Excessive lipophilicity, however, can lead to poor water solubility, making it difficult for the drug to dissolve in the aqueous environment of the GI tract for absorption, potentially limiting bioavailability

Sept. 15, 2024

Why small molecules are the best:

- Cell Membrane Barriers: Cell members, which separate the inside of cells from the external environment, are composed primarily of lipid (fat) bilayers. These bilayers act as selective barriers to molecules based on their size, charge, and solubility. The permeability of the membrane is governed by the lipophilicity of the molecules, meaning that fat-soluable substances can diffuse more easily across the lipid rich membrane

- Lipophilicity and diffusion: Smaller molecules are typically more lipophilic (fat soluble), allowing them to more easily pass through lipid based biological membranes (i.e. cell membranes). Polar groups create hydrogen bonds with water molecules, making the drug more hydrophilic (water soluable), which improves its ability to dissolve in the aqueous environment of the gastrointestinal tract. A small molecule have few

polar functional groups, just enough to strike a balance between hydrophilic and lipophilic, enabling the drug to be effectively absorbed in the intestines and distributed throughout the body.

- Hydrophilicity for distribution: Once absorbed, these small, slightly polar molecules can easily interact with the aqueous environment, and more easily be distributed throughout the body via the bloodstream to reach their target sites.

- Optimal size for targeting: Smaller molecules can often bind the the target receptors, protein, or enzyme more effectively due to their size and flexibility. Their smaller size enables them to fit better into the active sites of biological targets, enhancing their therapeutic effects.

② Log P value should be ≤ 5.

- Lipophilicity refers to the molecules ability to dissolve in fats or lipids, and log P quantifies this property.

- Too lipophilic (log P > 5):

- Poor solubility in water based environments like blood or gut fluids.
- Risk of accumulation in fatty tissues, leading to toxicity.

- Too hydrophilic (log P < 0):
- Excellent solubility in water, but poor membrane permeability, such molecules are unlikely to cross the hydrophobic lipid bilayer of cells, limiting absorption and effectiveness.

• For a drug to be absorbed orally, it must dissolve in the aqueous environment of the gastrointestinal (GI) tract (hydrophilic

and then cross the lipid bilayer of intestinal epithelial cells (lipophilicity?

- Optimal range ($\log P \leq 5$)

This range reflects the sweet spot where a molecule: (sufficiently soluble in both environments.)

Dissolves adequately in aqueous environments for transport in bloodstream and absorbtion in the gut

Can also partition into and cross lipid bilayers efficiently through passive difusion

Define?

⑤ $\leq$ 5 hydrogen bond donors
④ $\leq$ 10 hydrogen bond acceptors.

- Hydrogen bonds increase the molecules ability to interact with water, enhancing solubility in aqueous environment. Molecules with many hydrogen bond donors and hydrogen bond acceptors will readily dissolve in water, but struggle to cross into the hydrophobic lipid bilayer of membrane.

* These limits ensure that the molecule retains sufficient lipophilicity to cross cell membrane while maintaining enough hydrophilicity for water solubility.

Computer work logbook

Date	What was done ?
Sept. 1, 2024	Research all the common chronic disease. Make a table containing chronic disease name, what it does, what the treatment options are, what the adverse drug reactions are.
Sept 2, 2024	Compiled a list of all the adverse drug reaction.
Sept 3, 2024	Research the adverse drug reaction of medication used to treat adverse drug reactions of chronic disease treatments, their 3D structure was also obtained
Sept 4, 2024	Did the same
Sept 5, 2024	Did the same
Sept 6, 2024	Started research on the target protein involved in Adverse drug reaction, and ayurveda herb traditionally used. to treat the adverse drug reaction The target protein of adominal pain was researched, and so was the herb
	Target protein (cox 2) 3D structure was obtained.
Sept 9, 2024	The target protein of bloating was researched (Guanylate cyclase) and its 3D structure was retrieved the herb traditionally use was also researched.
Sept 10, 2024	Target protein of constipation was researched (Guanflate cyclase C), 3D structure was obtained, and herb traditionally used was researd.
Sept 11, 2024	The target protein of decreased appetite was researched (ghrelin receptor), and tradinally used herb was also researched.
Sept 12, 2024	The target protein of diarrhea was researched (serotonin receptor) and tradional herb was also researched.
Sept 13, 2024	Protein for heartburn ~~and~~ was researched (gastric proton pump) 3D structure was retrieved, and traditional herb used was researc

Sept. 14, 2024	Target protein involved in cough was research on its 3D structure was obtained The traditional herb used was also researched.
Sept 16, 2024	Target protin involved in difficulty breathing was researched (B_2AR receptor), its 3D structure was obtained, and herb was researched.
Sept. 17, 2024	Target protein involved in Pneumonitis was researched, 3D structure obtained (TNF-a receptor) and traditional herb was researched.
Sept. 18, 2024	Target protein involved in angioedema was researched, (B_2 receptor), 3D structure retrieved, and traditional herb researched.
Sept 19, 2024	Target protein involved in arrhythemia was researched ($Na_V1.5$), 3D structure was retrived and traditional herb was researched
Sept 20, 2024	Target protein involved in increased risk of blood clots was researched (Factor Xa), 3D structure was obtained, and traditional herb was researched.
Sept 21, 2024	Target protein involved in chest pain was researched (Troponin) 3D structure obtained and traditional herb was researched.
Sept. 22, 2024	Target protein involved in rapid heartbeat was researched (β_1 adrenergic receptor), 3D structure obtained, and tradional herb researched.
Sept 23, 2024	Target protein involved in high blood pressure was researched (ACE), 3D structure obtained, and tradional herb researched.
Sept 24, 2024	Target protein involved in low blood pressure was researched (Alpha 1 adrenergic receptor) was researched. 3D structure obtained, and traditionally

Sept 25, 2024	Target protein involved in leukopenia was researched (GCSF). 3D structure was retrieved, traditionally used herb was researched.
Sept 26, 2024	Target protein in blurred vision was researched (VEGF), 3D structure was obtained, traditonally used herbs was used
Sept 27, 2024	Target protein involved in fatigue was researched (A2A adenosine receptor), 3D structure obtained, and traditional herb was researched.
Sept 28, 2024	Target protein involved in hair loss was researched (5 alpha reductase enzyme), 3D structure obtained, and traditionally used herb was researched.
Sept 29, 2024	Target protein involved in joint pain was researched (TNF-a), 3D structure obtained, and traditionally used herb was researched.
Oct. 1, 2024	Target protein involved in muscle cramps was researched (RyR1) 3D structure was retrieved, and traditionally used herb was researched.
Oct. 2, 2024	Target protein involved in muscle weakness was researched (dystrophin), 3D structure was retrived, and traditionally used herb was researched.
Oct 3, 2024	Target protein involved in osteoporosis was researched (RANKL), 3D structure was retrieved, and traditionally used herb was researched.
Oct. 4, 2024	Target protein involved in fever was researched (Cox-2), 3D structure was retrieved, and tradionally used herb was researched.
Oct 5, 2024	Target protein involved in anxiety was researched (5-HT1A receptor) 3D structure was retrieved, and traditionally used herb was research

Oct 6, 2024	Target protein involved in depression was researched (5-HT1A), 3D structure was obtained, and traditionally used herb was researched.
Oct. 7, 2024	Target protein involved in insomnia was researched (GABA$_A$), 3D structure was obtained, and traditionally used herb was researched.
Oct. 8, 2024	To conduct molecular docking along with 3D structure of target proteins, 3D structure of bioactive compounds of ayurvedic herbs are also needed.
	Research was conducted to find all the bioactive compounds of triphala, 3D structures were retrieved and energy minimized and then molecular docking was conducted between all the bio active compounds of triphala and target protein COX-2.
Oct 9, 2024	Research was conducted to find all the bioactive compound of ajwain, 3D structures were obtained and energy-minimized and the molecular docking was conducted between all the bioactive compound of ajwain and target protein Guanylate Cyclase-C.
Oct 10, 2024	Research was conducted to find all the bioactive compounds of triphala, 3D structures were retrieved and energy minimized and then molecular docking was conducted between all the bioactive compounds of triphala and target protein Guanylate cyclase-C.
Oct. 11, 2024	Research was conducted to find all the bioactive compounds of chitrak, 3D structures were retrieved and energy minimized and then molecular docking was conducted between all the bioactive compounds of chitrak and target protein ghrelin receptor.

Oct. 12, 2024	Research was conducted to find all the bioactive compounds of lrael, 3D structures were retrived and energy minimized and then molecular docking was conducted between all the bioactive compounds of lrael and target protein 5-HT$_3$ receptor.
Oct 13, 2024	Research was conducted to find all the bioactive compounds of amla, 3D structures were obtained and energy minimized and then molecular docking was conducted between all the bioactive compounds of amla and target protein gastric proton pump
Oct. 14, 2024	Research was conducted to find all the bioactive compounds of tulsi, 3D structures were obtained and energy minimized and then molecular docking was conducted between all the bioactive compounds of tulsi and target protin TRPV1.
Oct. 15, 2024	Research was conducted to find all the bioactive compounds of pippali, 3D structures were obtained and energy minimized and then molecular docking was conducted between all the

Oct. 16, 2024	Research was conducted to find all the bioactive compounds of haridra, 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of haridra and target protein TNF
Oct. 17, 2024	Research was conducted to find all the bioactive compounds of turmeric, 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of turmeric and target protein B2 receptor
Oct. 18, 2024	Research was conducted to find all the bioactive compounds of arjuna, 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of arjuna and target protein Nav1.5.
Oct. 19, 2024	Research was conducted to find all the bioactive compounds of bibhitaki, 3D structures were obtained and energy minimization and then molecular docking was conducted between all bioactive compounds of bibhitaki and target protein (Gaba)
Oct. 20, 2024	Research was conducted to find all the bioactive compounds of arjuna, 3D structures

	were obtained and energy minimized, and then molecular docking was conducted between all the bioactive compounds of arjuna and target protein troponin I.
Oct. 21, 2024	Research was conducted to find all the bioactive compounds of arjuna, 3D structure were obtained and energy minimized and then molecular docking was conducted between all the bioactive compounds of arjuna and B1 receptor.
Oct. 22, 2024	Research was conducted to find all the bioactive compounds of arjuna, 3D structure were obtained and energy minimized and then molecular docking was conducted between all the bioactive compounds of arjuna and ACE
Oct. 23, 2024	Research was conducted to find all the bioactive compounds of ashwagandha, 3D structures were obtained and energy minimized and then molecular docking was conducted between all the bioactive compounds of ashwagandha and target protein Alpha 1 adrogenic receptor.

Oct. 24, 2024	Research was conducted to find all the bioactive compounds of guduchi, 3D structures were obtained and energy minimized and then molecular docking was conducted between all the bioactive compounds of guduchi on target protein G-CSF
Oct. 25, 2024	Research was conducted to find all the bioactive compounds of amla, 3D structures were obtained and energy minimized and then molecular docking was conducted between all the bioactive compounds of amla and target protein VEGF.
Oct. 26, 2024	Research was conducted to find all the bioactive compounds of ashwagandha, 3D structures were obtained and energy minimized and then molecular docking was conducted between bioactive compounds of ashwagandha and target protein A2A adenosine receptor
Oct. 27, 2024	Research was conducted to find all the bioactive compounds of bhringraj, 3D structures were obtained and energy minimized and then molecular docking was conducted between bioactive compounds of bhringraj and target protein 5 alpha reductase enzyme.

Oct. 28, 2024	Research was conducted to find all the bioactive compounds of shallaki, 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of shallaki and target protein 5-LOX.
Oct. 29, 2024	Research was conducted to find all the bioactive compounds of nirgundi, 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of nirgundi and target protein RyR1.
Oct. 30, 2024	Research was conducted to find all the bioactive compounds of ashwagandha, 3D structures were retrieved and energy minimized and then molecular docking was conducted between all the bioactive compounds of ashwagandha and target protein Dystrophin.
Nov. 1, 2024	Research was conducted to find all the bioactive compounds of haldi, 3D structures were retrieved and energy minimized and then molecular docking was conducted between all bioactive compounds of haldi and target protein RANKL
Nov. 2, 2024	Research was conducted to find all the bioactive compounds of giloy, 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of giloy and target protein COX-2.
Nov. 3, 2024	Research was coducted to find all the bioactive compounds of ashwagandha, 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of ashwagandha and target 5-HT1A.
Nov. 4, 2024	Research was conducted to find all the bioactive compounds of tagara; 3D structures were obtained and energy minimized and then molecular docking was conducted between all bioactive compounds of tagara and target protein GABA(a)
Nov. 7, 2024	To compare we also needed molecular docking scores of conventional drugs to treat adverse drug reactions, and we already obtained the 3D structures while researching earlier.

Nov. 8, 2024	Molecular docking of conventional drugs and target proteins.
Nov. 9, 2024	same thing
Nov 10, 2024	same thing
Nov. 11, 2024	same thing
Nov. 12, 2024	same thing
Nov. 13, 2024	same thing
Nov. 14, 2024	Bioactive compounds ~~of~~ with highest molecular docking scores where checked for oral bioavailability using lipinskis rule of five.
Nov 15, 2024	same thing
Nov. 16, 2024	same thing
Nov. 17, 2024	same thing
Nov 18, 2024	same thing
Nov 19, 2024	same thing
Nov 20, 2024	same thing
Nov. 21, 2024	same thing
Nov. 22, 2024	same thing
Nov. 23, 2024	same thing
Nov. 24, 2024	same thing
	PDF
Nov. 28, 2024	With this step the methodology ended and I started on the actual research