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In Silico Insights into *Amalaki*: Computational Profiling of Drug-Like Potentials of *Emblica officinalis*

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KEYWORDS

Emblica officinalis, Amalaki, Druglikeness, Lipinski's Rule, Bioavailability.

ABSTRACT:

The study explores the drug-likeness of phytochemicals derived from *Emblica officinalis* (Amla), a medicinal herb that is frequently employed in Ayurvedic and Unani traditional treatment systems. Well-known for its anti-inflammatory, anti-cancer, hepatoprotective, and antioxidant qualities, E. *officinalis* contains numerous bioactive compounds like flavonoids, tannins, and glycosides. Utilizing computer-aided drug design (CADD) tools, this research aims to evaluate the potential of these phytochemicals as viable drug candidates based on their physicochemical properties. Fifty selected phytochemicals were analyzed using canonical SMILES obtained from the PubChem database. ChemDraw was used to create chemical structures, and the MolSoft web server was used to predict drug-likeness scores using Lipinski's Rule of Five as the main screening criterion. Molecular weight (<500 Da), lipophilicity (ClogP <5), hydrogen bond donors (<5), and hydrogen bond acceptors (<10) are the criteria used by the rule to evaluate drug-likeness. Out of the 50 compounds evaluated, 30 met the drug-likeness criteria, showing promising profiles for oral bioavailability and therapeutic development. Nineteen compounds failed the criteria—five had two violations and fourteen had three violations—implying lower likelihood of oral activity. Tannic acid was excluded from the final analysis due to incomplete data from the software. The results demonstrate the efficacy of in silico tools in rapidly screening natural products for drug development. By merging traditional knowledge with modern computational approaches, this research underlines the potential of *E. officinalis* as a rich source of novel bioactive compounds. It is advised that more experiments be conducted to validate these results and get particular phytochemicals closer to medicinal uses. This study contributes to natural product-based drug discovery by identifying candidates suitable for further pharmacological development.

INTRODUCTION:

The medicinal plant Emblica officinalis is widely used in traditional medical systems such as Ayurveda, Unani, and traditional Chinese medicine, also referred to as *Amalaki*. The fruit of *Emblica officina*lis is highly valued for its many medicinal qualities, which include hepatoprotective, anti-inflammatory, anti-microbial, antioxidant, and anticancer activities. Its high phytochemical content—which contains triterpenoids, flavonoids, glycosides, and tannins—is responsible for these benefits [1]. A molecule must have favourable drug-like qualities including solubility, permeability, and bioavailability in order to be regarded as a promising drug candidate. For the molecule to reach the intended location in the body at therapeutic concentrations, several characteristics are essential [2]. Drug-likeness is frequently predicted using Lipinski's Rule of Five, which considers variables like molecular weight, donors and acceptors of hydrogen bonds, and the octanol-water

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partition coefficient (logP). In general, compounds are regarded as less likely to be orally active medications if they fail to meet more than one of these requirements [3]. Computer-Aided Drug Design (CADD) is the term for the incorporation of computer tools in drug discovery, which has greatly improved the process's efficiency. Using techniques like pharmacophore modeling, molecular docking, and Quantitative Structure-Activity Relationship (QSAR) modelling [4], researchers can rapidly assess and optimize potential drug candidates. In addition to speeding up the drug development process, these computational techniques increase the precision of forecasting a compound's drug-like characteristics and possible therapeutic efficacy [5]. *Emblica officinalis* has been shown to contain phytochemicals such quercetin, gallic acid, ellagic acid, chebulagic acid, and chebulinic acid. These substances are promising candidates for therapeutic development since they have shown a variety of biological actions, such as anti-inflammatory, antioxidant, and anticancer properties. possible candidates for the creation of new drugs. However, the assessment of their drug-like qualities by computational approaches is necessary to determine their feasibility as drug candidates. Numerous databases and computational techniques are available for predicting the drug-like properties of phytochemicals. Topological Polar Surface Area (TPSA), molecular weight, logP, and bioavailability are some of the attributes that are commonly predicted using SwissADME, Molinspiration, and PreADMET [6].

We should concentrate on combining experimental validation with computational predictions to improve the drug discovery process for phytochemicals found *in Emblica officinalis*. Drug discovery could greatly benefit from the use of computational techniques to forecast the drug-like characteristics of phytochemicals derived from *Emblica officinalis*. These techniques provide important insights into the therapeutic potential of possible drug candidates while enabling quick screening and optimization. Nevertheless, additional investigation is required to confirm these hypotheses and convert them into potent medicinal substances.

In this work, we use sophisticated computational methods to forecast the drug-like characteristics of certain phytochemicals that are extracted from *Emblica officinalis*. This method highlights the compounds' aptitude for additional development and optimization while offering insightful information about their potential as therapeutic candidates. The use of computer techniques to assess the phytochemicals of *Emblica officinalis* highlights the increasing significance of in silico tools in contemporary drug discovery. This study aims to find prospective drug-like candidates from *Emblica officinalis* by fusing traditional knowledge with state-of-the-art technology. This will help to advance the area of natural product-based drug discovery and open the door to new therapeutic advancements.

MATERIALS AND METHODS:

Canonical smiles are gathered and SDF files are downloaded using the Pubchem database. Drug likeness is determined using Molsoft software.

Phytochemicals List:

The list of selected phytochemicals included in the study are, Procyanidin(bark), Proanthocyanidin, Tannic acid(bark), Leucodelphidin, Lupeol(bark), Pyrogallol, 1,3,6-tri-O-galloyl-beta-D-glucose, Riboflavin(fruit), Furosin, Terchebin, Phloroglucinol, trans-Zeatin, Quercetin, Chebulagic acid(fruit), Ellagic acid(fruit), Methyl gallate, Ascorbic acid(fruit), Kzeyiyxacmutrm-uhfffaoysa-, Phyllantidine(fruit), Ethyl gallate, beta-Glucogallin, Galactaric acid(fruit), Chebulinic acid(fruit) [7], Corilagin(fruit), Chebulic acid(fruit), Geraniin(fruit), Trigalloylglucose, Tryptase, Terchebin, Kaempferol, Astragalin, beta-Sitosterol(leaf), Oleanolic aldehyde, Epigallocatechin gallate, Oleanolic acid, Myristic acid, Stearic acid, Palmitic acid, Nicotinic acid, alpha-Carotene, Oleic acid, Linolenic acid(seed), D-Glucose, D-Galacturonic Acid(seed), Linoleic acid(stem), Eriodictyol-7-O-glucoside, 2-Methoxycarbonyl-6-oxo-3-[2,3,4-trihydroxy-6-[4-hydroxy-6-(hydroxymethyl)-2-(3,4,5-trihydroxybenzoyl) oxyoxan-3-yl] oxycarbonylphenyl] oxane-4-carboxylic acid, Inositol, beta-Carotene. Total of 88 phytochemicals were identified from the PubChem database and out of them only 50 were used for current study. Remaining phytochemicals were omitted because some of the phytochemicals are repeated more often [8][9][10].

List SMILES of Phytochemicals from PubChem Database:

We visited the PubChem website and utilized the search box to look up each phytochemical by name in order to compile SMILES for certain phytochemicals. We clicked on the compound to view its compound summary page after finding it in the search results. Upon navigating to the "Chemical and Physical Properties"

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section, we came across the " SMILES" field, which is normally located under "Molecular Descriptors." We then copied the standard SMILES string and repeated this process for each phytochemical [11].

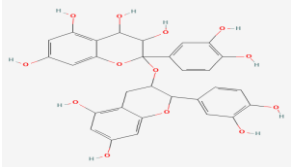
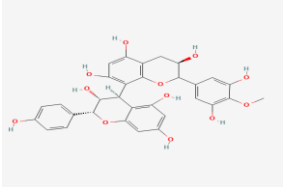
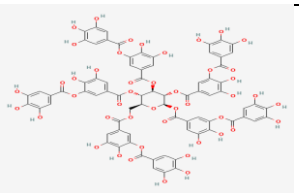
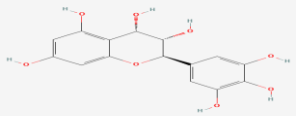
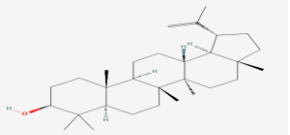
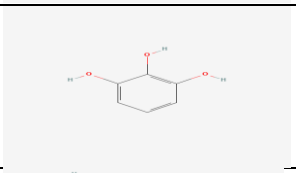
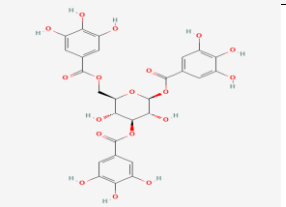
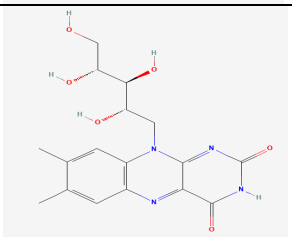
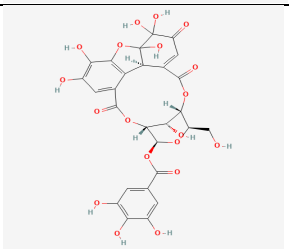
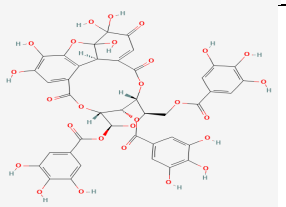
ChemDraw structures of selected phytochemicals:

Using a canonical SMILES string, we have illustrated the chemical structures of specific phytochemicals using ChemDraw's "Structure" feature. Then, after selecting "Convert SMILES to Structure" and entering the canonical SMILES string into the resulting input box, we selected "OK". The automatically generated structure can be altered using ChemDraw's capabilities, such as the bond and atom tools. Table 1 displays the chemical structure of a few selected phytochemicals [12].

Determination of Drug Likeness Score:

MolSoft web servers (https://molsoft.com/mprop/) were used to forecast the drug-like characteristics of phytocompounds [13]. Lipinski's rule of five, which states that molecules should have a molecular weight of 500, a C logP of 5, less than five hydrogen bond donors, and fewer than ten hydrogen bond acceptors, was used to determine drug-like qualities [14]. To forecast drug-like properties of compounds, the standard Simplified Molecular Line-Entry Systems (SMILES) were acquired from PubChem and entered into the MolSoft web server [15][16][17][18].

Table 1: Chemical structure of selected phytochemicals.

SL .NO	PHYTOCHEMICALS	CHEM DRAW STRUCTURE
1	Procyanidin(bark)	
2	Proanthocyanidin	
3	Tannic acid(bark)	
4	Leucodelphidin	
5	Lupeol(bark)	
6	Pyrogallol	
7	1,3,6-tri-O-galloyl-beta-D-glucose	
8	Riboflavin(fruit)	
9	Furosin	
10	Terchebin	

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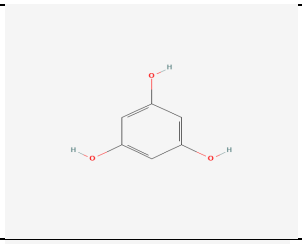
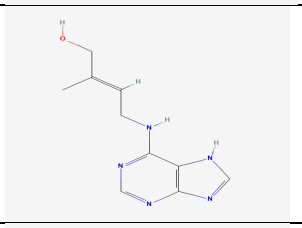
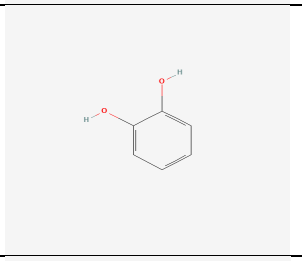
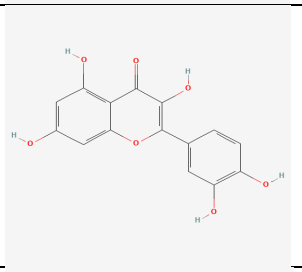
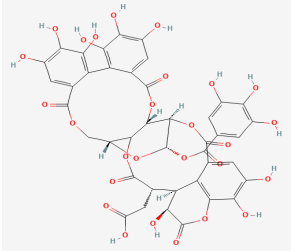
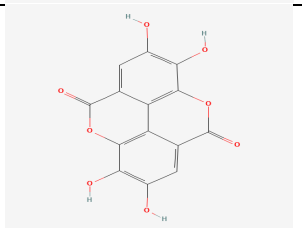
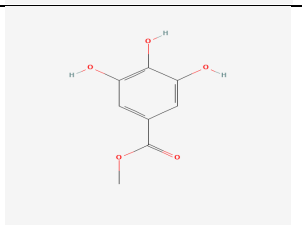
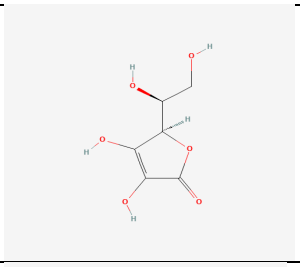
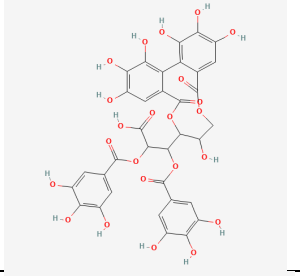
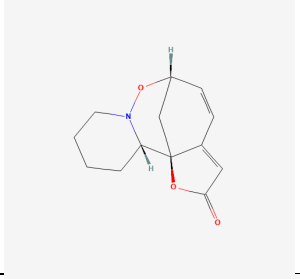
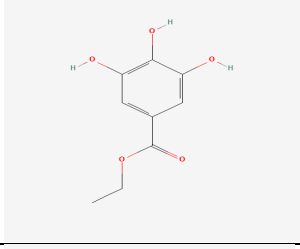
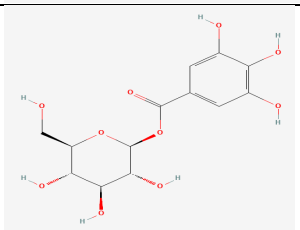
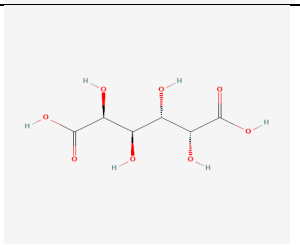
11	Phloroglucinol	
12	trans-Zeatin	
13	Catechol	
14	Quercetin	
15	Chebulagic acid(fruit)	
16	Ellagic acid(fruit)	
17	Methyl gallate	

18	Ascorbic acid(fruit)	
19	Kzeyiyxacmutrm-uhfffaoysa-	
20	Phyllantidine(fruit)	
21	Ethyl gallate	
22	beta-Glucogallin	
23	Galactaric acid(fruit)	

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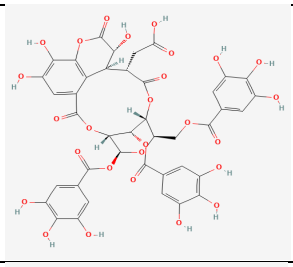
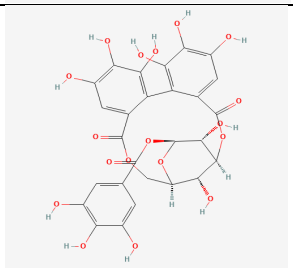
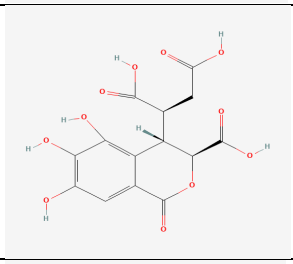
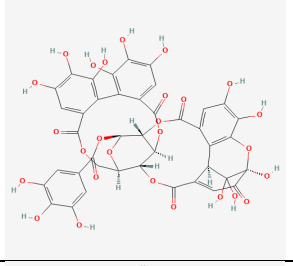
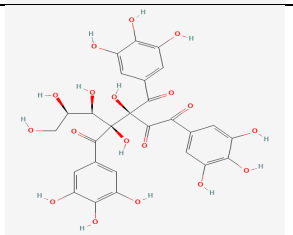
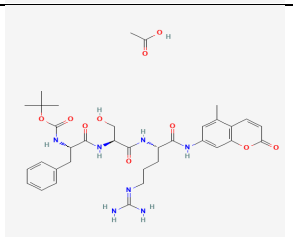
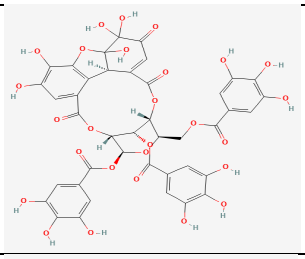
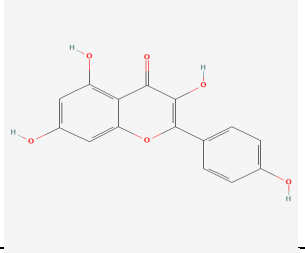
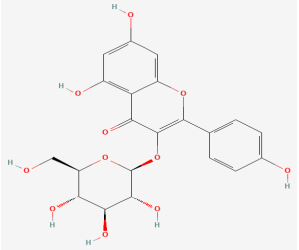
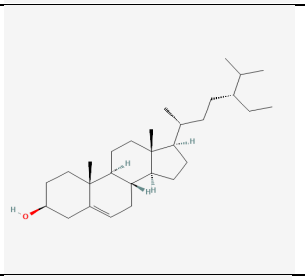
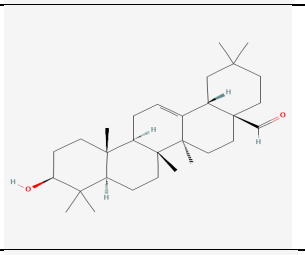
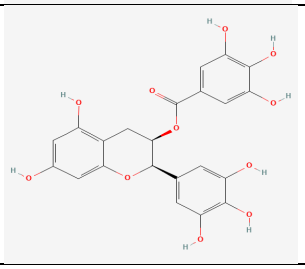
24	Chebulinic acid(fruit)	
25	Corilagin(fruit)	
26	Chebulic acid(fruit)	
27	Geraniin(fruit)	
28	Trigalloylglucose	
29	Tryptase	

30	Terchebin	
31	Kaempferol	
32	Astragalin(leaf)	
33	beta-Sitosterol(leaf)	
34	Oleanolic aldehyde	
35	Epigallocatechin gallate	

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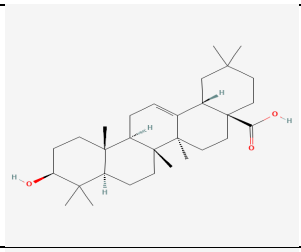
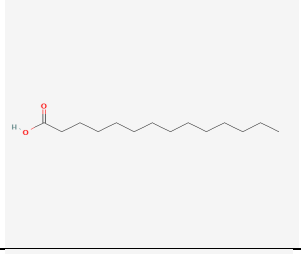
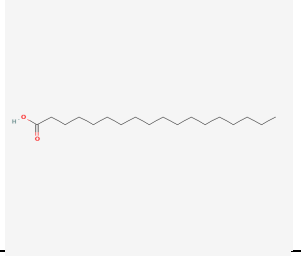
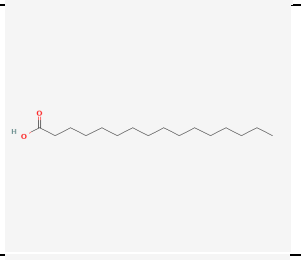
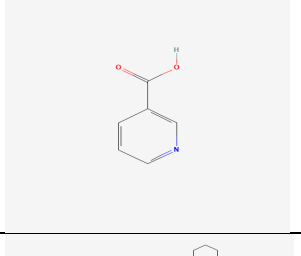
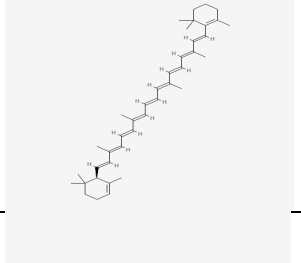
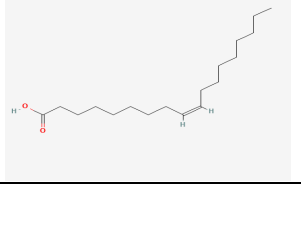
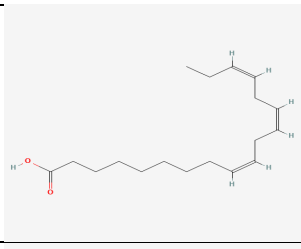
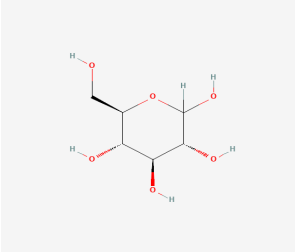
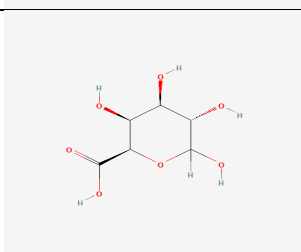
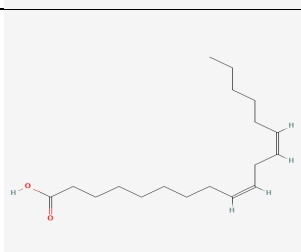
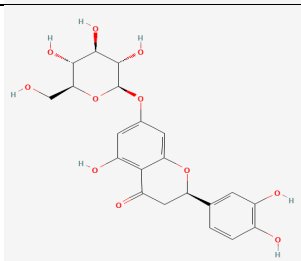
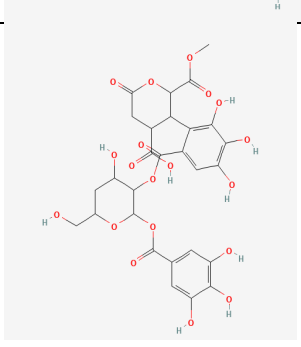
36	Oleanolic acid	
37	Myristic acid	
38	Stearic acid	
39	Palmitic acid	
40	Nicotinic acid(seed)	
41	alpha-Carotene	
42	Oleic acid	

43	Linolenic acid(seed)	
44	D-Glucose	
45	D-Galacturonic Acid(seed)	
46	Linoleic acid(stem)	
47	Eriodictyol-7-O-glucoside	
48	2-Methoxycarbonyl-6-oxo-3-[2,3,4-trihydroxy-6-[4-hydroxy-6-(hydroxymethyl)-2-(3,4,5-trihydroxybenzoyl) oxyoxan-3-yl] oxycarbonylphenyl] oxane-4-carboxylic acid	

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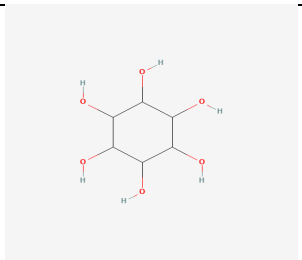
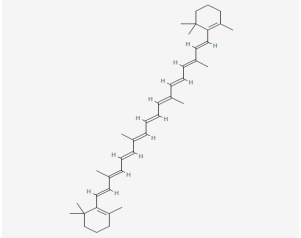
49	Inositol	
50	beta-Carotene	

Table 2: Drug Likness Profile of Phytochemicals from *Emblica officinalis*.

SL .NO	PHYTO CHEMICALS	Molecular weight <500	ClogP <5	HBA <10	HBD <5	DLS <1	Number of violations <1
1	Procyanidin(bark)	594.14	1.63	13	10	0.91	3
2	Proanthocyanidin	592.16	2	12	9	0.86	3
3	Tannic acid(bark)	-	-	-	-	-	-
4	Leucodelphidin	322.07	-0.03	8	7	-0.06	1
5	Lupeol(bark)	426.39	8.35	1	1	-0.22	1
6	Pyrogallol	126.03	0.93	3	3	-1.36	0
7	1,3,6-tri-O-galloyl-beta-D-glucose	636.1	-0.08	18	11	0.92	3
8	Riboflavin (fruit)	376.14	-1.5	8	5	0.62	0
9	Furosin	650.08	-1.29	19	10	0.8	3
10	Terchebin	954.1	0.26	27	14	0.57	3
11	Phloroglucinol	126.03	0.31	3	3	-1.05	0
12	trans-Zeatin	219.11	1.11	4	3	-0.88	0
13	Catechol	110.04	1.2	2	2	-1.44	0
14	Quercetin	302.04	1.19	7	5	0.52	0
15	Chebulagic acid(fruit)	954.1	0.22	27	13	0.58	3
16	Ellagic acid(fruit)	302.01	1.53	8	4	-1.11	0
17	Methyl gallate	184.04	0.9	5	3	-0.65	0
18	Ascorbic acid(fruit)	176.03	-1.59	6	4	0.74	0
19	Kzeyiyxacmutrm-uhfffaoysa-	802.09	0.38	23	14	0.26	3
20	Phyllantidine(fruit)	233.11	1.85	4	0	-1.03	0
21	Ethyl gallate	198.05	1.4	5	3	-0.39	0
22	beta-Glucogallin	332.07	-1.9	10	7	0.81	0
23	Galactaric acid(fruit)	210.04	-3.75	8	6	0.59	0
24	Chebulinic acid(fruit)	956.11	-0.36	27	13	0.7	3
25	Corilagin(fruit)	634.08	0.51	18	11	0.64	3
26	Chebulic acid(fruit)	356.04	-1.27	11	6	-0.29	2
27	Geraniin(fruit)	952.08	0.61	27	14	0.3	3
28	Trigalloyl glucose	636.1	-2.07	18	14	0.3	3
29	Tryptase	725.34	1.91	11	10	-1.14	3
30	Terchebin	954.1	0.26	27	14	0.57	3
31	Kaempferol	286.05	1.61	6	4	0.5	0
32	Astragalin (leaf)	448.1	-0.12	11	7	0.67	2
33	beta-Sitosterol(leaf)	414.39	8.45	1	1	0.78	1
34	Oleanolic aldehyde	440.37	6.96	2	1	-0.16	1
35	Epigallocatechin gallate	458.08	1.44	11	8	0.23	2
36	Oleanolic acid	456.36	6.66	3	2	0.37	1
37	Myristic acid	228.21	5.63	2	1	-0.54	1
38	Stearic acid	284.27	7.65	2	1	-0.54	1
39	Palmitic acid	256.24	6.64	2	1	-0.54	1
40	Nicotinic acid(seed)	123.03	0.51	3	1	0.3	0
41	alpha-Carotene	536.44	14.34	0	0	0.37	2
42	Oleic acid	282.26	7.11	2	1	-0.3	1
43	Linolenic acid(seed)	278.22	5.88	2	1	0.09	1
44	D-Glucose	180.06	-3.02	6	5	-0.12	0
45	D-Galacturonic Acid(seed)	194.04	-2.97	7	5	-0.3	0

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46	Linoleic acid(stem)	280.24	6.6	2	1	-0.3	0
47	Eriodictyol-7-O-glucoside	450.12	-0.31	11	7	0.91	1
48	2-Methoxycarbonyl-6-oxo-3-[2,3,4-trihydroxy-6-[4-hydroxy-6-(hydroxymethyl)-2-(3,4,5-trihydroxybenzoyl)oxyoxan-3-yl]oxycarbonylphenyl]oxane-4-carboxylic acid	668.12	-1.36	19	9	0.83	3
49	Inositol	180.06	-3.1	6	6	-0.89	1
50	beta-Carotene	536.44	13.93	0	0	0.64	2

RESULTS:

Drug-likeness" is a term used in pharmaceutical research to describe how similar a compound is to known, successful drugs. It involves analyzing whether a compound has the kinds of physical and chemical characteristics typical of molecules that become effective drugs. A major factor here is oral bioavailability, meaning whether the compound can be effectively absorbed when taken by mouth. To assess drug-likeness, scientists use various metrics, especially Lipinski's Rule of Five.

Lipinski's Rule of Five (RO5)

Christopher A. Lipinski created this set of rules to assess a chemical compound's likelihood of making an effective oral medication for people. The reason it is known as the "Rule of Five" is that the values are derived from multiples of five. The rule states that a substance has a higher chance of being orally bioavailable if it satisfies the following requirements: Molecular Weight (MW) < 500 Daltons → Smaller molecules are generally easier for the body to absorb. Hydrogen Bond Donors (HBD) ≤ 5 → These are atoms like OH or NH groups that donate hydrogen bonds. Too many make it harder to cross cell membranes. Hydrogen Bond Acceptors (HBA) ≤ 10 → These are atoms like oxygen or nitrogen that accept hydrogen bonds. Partition Coefficient (Log P) ≤5 → These measures how soluble the compound is in fats vs. water. Balanced solubility helps absorption. No more than one violation of the above rules → More than one violation typically suggests poor bioavailability [19].

88 phytochemicals were originally identified from a plant specimen., However, only 50 were chosen for evaluation because some compounds were repeated across multiple parts of the plant (like leaf, root, bark, fruit), and duplicates were removed to avoid redundancy. Analysis of the 50 Phytochemicals The compounds were analyzed using physicochemical criteria (MW, HBA, HBD, Log P) and Lipinski's Rule of Five. The MolSoft web server was used for this analysis—a computational tool that predicts a molecule's "druggability" or potential to become a drug.30 of the 50 compounds passed the Lipinski criteria, indicating they have good drug-like properties.19 compounds violated Lipinski's Rule:5 compounds had two violations, 14 compounds had three violations, This means those 19 compounds are less likely to be orally bioavailable, and therefore, less promising as drug candidates. 30 phytochemicals (Leucodelphidin, Lupeol(bark), Pyrogallol, Riboflavin, Phloroglucinol, trans-Zeatin, Catechol, Quercetin, Ellagic acid, Methyl gallate, Ascorbic acid(fruit), Phyllantidine(fruit), Ethyl gallate, beta-Glucogallin, Galactaric acid, Kaempferol, beta-Sitosterol, Oleanolic aldehyde, Oleanolic acid, Myristic acid, Stearic acid, Palmitic acid, Nicotinic acid, Oleic acid, Linolenic acid(seed), D-Glucose, D-Galacturonic Acid , Linoleic acid, Eriodictyol-7-O-glucoside, Inositol) appear promising as potential oral drug candidates. During the research for phytochemicals in PubChem tannic acid's chemical structure was derived from it but an error appeared while trying to get the MW, HBD, HBA and DLS values from MolSoft software. Those values were not retrieved and presented in the table 2. These can be further investigated for their effects against specific diseases. The study uses Lipinski's Rule as a fundamental screening tool to filter out less viable compounds early in the drug discovery process.

DISCUSSION:

The idea of "drug likeness," which describes how closely a chemical resembles the properties of a conventional drug, especially in terms of bioavailability, is essential to drug design. In order to learn more about the bioavailability of specific phytochemicals in the

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human body, a number of drug-related metrics were calculated for them. Finding out if these phytoconstituents have qualities that make them good candidates for medication development was the main goal of the study.

During the search for phytochemicals a total of 88 phytoconstituents were found in the plant specimen. Among them 50 phytochemicals were scrutinized because of repetition of the same phytoconstituent 2 or more times. Same phytochemicals are found in leaf, root, bark as well as fruits etc. Among the 50 phytochemicals the 30 of them showed drug like properties that followed the Lipinski's rule of 5. 19 phytochemicals showed violations of the Lipinski's rule (5 of them had 2 violations and 14 of them had 3 violations). This indicates that there are total of 30 phytochemicals have druglike properties which can be further studied for their effectiveness in specific diseases. A well-known framework in drug design, Lipinski's Rule of Five uses a compound's physicochemical characteristics to determine how drug-like it is. In general, it is believed that drugs that contravene more than one of these rules are less likely to be orally active. The majority of the chosen phytochemicals from *Emblica officinalis* met Lipinski's criteria, according to the study's analysis, indicating that they may make good therapeutic candidates. However, certain phytochemicals showed several infractions of these guidelines, suggesting that more work may be required to enhance their oral bioavailability and general drug-likeness. The study's findings have significant ramifications for the creation of novel medications made from natural sources, particularly phytochemicals found in *Emblica officinalis*. An efficient and affordable way to find possible drug candidates is to use computational methods to anticipate drug-likeness, which eliminates the need for more expensive experimental procedures in the early stages. Numerous assessed phytochemicals satisfied the drug-likeness requirements, indicating their potential for additional research as medicinal agents.

CONCLUSION:

Fifty phytoconstituents that were isolated from Emblica officinalis were thoroughly analyzed in order to evaluate their physicochemical characteristics and drug-likeness. According to Lipinski's rule of five, the results showed that a sizable percentage of these phytoconstituents had favorable drug likeness. Their physicochemical characteristics also came within the recommended ranges, indicating the highest levels of membrane permeability and bioavailability. These findings clearly imply that *Emblica officinalis* phytoconstituents have a great deal of promise as possible medicinal agents. Their good physicochemical characteristics and adherence to Lipinski's rule of five underscore their appropriateness for additional investigation and advancement in pharmaceutical research, highlighting their encouraging potential for successfully treating a range of medical diseases.

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