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Identification and In-Silico Profiling of Phytoconstituents in Leaves of *Punica grantum* L.

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ABSTRACT

Punica granatum L. also called Pomegranate, a valuable fruit belonging to Punicaceae family. Pomegranate is not only nutrious but has remarkable medicinal properties. This study aimed to identify the phytochemical constituents present in Pomegranate leaves utilizing Gas Chromatography-Mass Spectrometry (GC-MS) technique, and to assess their medicinal potential using the PASS online software. The results of the analysis revealed the presence of several important phytochemicals, like Neophytadiene,Phytol,1,2 Benzene Dicarboxylic acid known for their medicinal properties such as Saccharopepsin inhibitor, Retinol dehydrogenase inhibitor, anti-inflammatory, anti-pyretic and anti-cancer. From the screened potent compounds, notably Phytol showed good activity which can be further evaluated for in-vivo drug evaluation. This study contributes to the understanding of the phytochemical composition and medicinal potential of Pomegranate leaves, highlighting its significance as a valuable natural resource for pharmaceutical research and development.

Keywords : Punica granatum L.,GC-MS, Phytol, Saccharopepsin inhibitor

I. INTRODUCTION

Punica granatum L. also known as Pomegranate is an healthy and economically important fruit plant belonging to family Punicaceae. It has been noted that Iran, Turkey, Greece, Armenia, Egypt, Palestine, Tunisia, India, Afghanistan, China, Japan, Morocco, Spain, France, Cyprus, and Italy are the most important countries around the world which produce pomegranate[1]. Pomegranate is additionally essential

in human medicine and its components have extensive range of clinical applications[2].

GC-MS, or gas chromatography mass spectrometry, is a potent analytical method for locating and measuring organic compounds in complicated mixtures. It blends the detection and identification powers of mass spectrometry with the separation capabilities of Gas chromatography[3]

Pass is computer based software that provides information about biological activity of chemical compound based on their chemical structure[4]. The current version of PASS can predict more than 3750 biological activity [5]. with accuracy level of 95%. The prediction is based on probability; probable active (pa) and probable inactive (Pi)[6]. Chemical compound is considered potent if the value of Pa>Pi. Greater the pa value ,more the potent chemical compound, Compound having pa value less than 0.7 have less probability of observing the activity [5].

This study mainly focuses on metabolite investigation in leaf extract of Punica granatum L. using GC-MS and prediction of its pharmacological activity using Pass online server.

II. METHODS AND MATERIAL

2.1 Preparation of Plant Extract

20g of Punica granatum L. leaves powder was macerated with 200 ml of n- hexane for 8 hours and than sample were extracted using soxhlet extraction method for 8 hours at 50-60 C. Extracts were filtered and diluted to appropriate concentration and used for used for Gas chromatography mass spectrometry analysis.

2.2 Gas chromatography mass spectrometry analysis in leaves of Punica granatum L.

Phytochemical analysis for hexane extract was carried out using shimadzu QP 2010 GC consisting of auto sampler and hyphenated with mass spectrometer. For GC-MS detection, BPX (Cyanopropyl Polysilphenylene-siloxane) capillary column of (30 × 0.53 ID × 3 μm df) was used. For ionization in mass spectrometer, electron ionization method was used with ionization energy of 70eV. Helium gas at flow rate of 1.4 mL/min was used as carrier gas and 2 μL sample was injected in split mode for the analysis. The ion source temperature was maintained at 230˚C, injector temperature at 250˚C. Mass spectra were taken at 70 eV; a scan interval of 0.5 s and fragments from 60 to 1000 Da. The solvent delay was 0 to 2 min, and the total GC/MS running time was 26 min. Blank peaks were eliminated from the sample. Interpretation of the obtained peaks in spectrum was carried out using database and obtained unknown peaks were compared with Wiley,NIST11 and NIST 11s library with results indicating name, molecular weight, and structure of the components. Percentage of each component was calculated by comparing its area with total area.

2.3 Biological activity Prediction of Phytoconstituents using PASS online software.

In silico activity prediction of selected phytoconstituents identified by GC-MS was done using Pass online server(www.way2drug.com) [7-8]. It reveals the prediction score for biological traits by means of ratio of probability to be active Pa to the probability to be inactive Pi. Enhanced value of Pa indicates higher probability of a given biological activity for the component.

III. RESULTS AND DISCUSSION

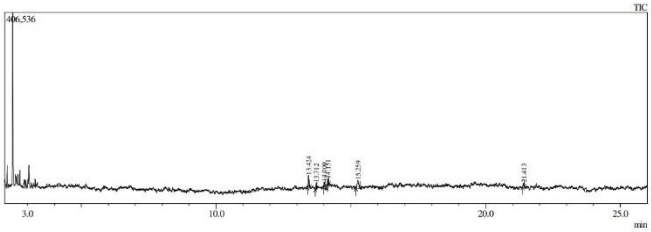

Fig.1 : GC chromatogram of Punica granatum L. leaf hexane extract

Table-1 Phytoconstituents present in leaves of healthy Punica granatum L. hexane extract

Sr. no	Retention time (min)	Relative percentage	Compound name
1.	13.42	19.52	Neophytadiene
2.	13.71	9.28	Phytol
3.	14.00	11.62	1,2-Benzenedicarboxylic acid
4.	14.15	6.28	Hexadecanoic acid
5.	15.25	41.05	Linoleic acid chloride
6.	21.41	12.25	Farnesyl acetone

Results of GC-MS analysis revealed presence of important phytochemicals like Neophytadiene , 1,2-Benzenedicarboxylic acid and Linoleic acid chloride. Hexadecanoic acid exerts anti-inflammatory action by inhibiting phospholipase A2 2 [9.10] .Hexadecanoic acid also posses anti-bacterial, anti-fungal, anti-oxidant, anti-psychotic and anti-androgenic [11,12] . Octadecanoic acid is anti-bacterial, anti-fungal and anti-tumor activities [13]. It is employed as solidifying agent in cosmetic formulations [14].

Table- 2 : In-silico activity prediction of phytoconstituents of Punica granatum L. using Pass online server

Compound Name	Pa	Pi	Activity
Neophyatadiene	0.863	0.014	Phobic disorder treatment
	0.853	0.014	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
	0.853	0.019	Aspulvinone dimethylallyltransferase inhibitor
	0.833	0.014	Saccharopepsin inhibitor
Palmitic acid	0.973	0.001	Acylcarnitine hydrolase inhibitor
	0.962	0.002	CYP2J substrate
	0.954	0.001	Carboxypeptidase Taq inhibitor
	0.933	0.004	Mucomembranous protector
Phytol	0.911	0.002	Prenyl-diphosphatase inhibitor
	0.905	0.005	Ubiquinol-cytochrome-c reductase inhibitor
	0.893	0.007	Phobic disorder treatment
	0.852	0.009	Mucomembranous protector
	0.845	0.012	Chymosin inhibitor

Phytol possess antinoconceptive, anti-oxidant, antimicrobial, anti-cancer, anxiolytic, anti-depressant, anti-inflammatory, anti-hyperalgesic, anti-pyretic and anti-arthritic activities [15,16] . It also aids healing of headache, rheumatism and some skin ailments [17]. Phytol possess antinoconceptive, anti-oxidant, anti-microbial, anti-cancer, anxiolytic, anti-depressant, anti-inflammatory, anti- hyperalgesic, anti-pyretic and anti-arthritic activities [18,19]. Phytol is used as incense substance and is incorporated in variety of cosmetic and non-cosmetic formulations [20]

Phytol, chlorophyll derived diterpene alcohol is a optimistic antischistosomal agent as a remedy for Schistosomiasis [21]. Neophytadiene possesses analgesic, anti-microbial, antipyretic, anti-inflammatory and anti-oxidant characteristics [22]. Phytol, phytol acetate, neophytadiene and Oxacycloheptadec-8-en-2-one also depicted saccharopepsin inhibitor activity (Pa>0.7).Variation in extent of activity Saccharopepsin (Proteinase A) is associated with inception of hypertension, gastric ulcers and neoplastic diseases [23]

IV.CONCLUSION

The term Phytochemicals that are plant based chemicals was introduced to all over the world in 1994 and became highly popular for researchers and scientists due to their various therapautic advantages. Punica granatum L. commonly known as pomegranate possess various health beneficial applications like anti cancer, anti-inflammatory, protection agianst alzheimer disease. In present study preliminary phytochemical screening and identification of phytochemicals present in leaves of pomegranate was carried out using GC-MS technique and identified phytochemicals were subjected to computed software pass online for therapautic potential. Results of analysis revealed presence of highly beneficial phytoconstituents like phytol and neophytadiene posssesing resistance for phobic disorder treatment also leaf extracts may be utilized for therapeutics like anti - inflammatory,anti cancer ,anti-hypercholesterolemic and antiprotozoal drugs.

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VI. REFERENCES

[1]. Stover, E. D., & Mercure, E. W. (2007). The pomegranate: a new look at the fruit of paradise. HortScience, 42(5), 1088-1092.

[2]. Sarkhosh, A., Zamani, Z., Fatahi, R., & Ebadi, A. (2006). RAPD markers reveal polymorphism among some Iranian pomegranate (Punica granatum L.) genotypes. Scientia Horticulturae, 111(1), 24-29.

[3]. Smith, J. A., & Johnson, B. C. Gas Chromatography Mass Spectrometry: Principles and Application.

[4]. Sharma, M. N. (2018). Identification of molecular targets of potential antidiabetic drugs using prediction of activity spectra for substances and molecular docking. International Journal of Green Pharmacy (IJGP), 12(02).

[5]. Habibyar, A. F., Sharma, N., & Khurana, N. (2016). PASS assisted prediction and pharmacological evaluation of hesperidin against scopolamine induced amnesia in mice. European Journal of Pharmacology, 789, 385-394.

[6]. Kumar, R., Kumar, R., Anand, A., Sharma, N., & Khurana, N. (2018). Prediction of anti-parkinson potential of phytoconstituents using prediction of activity spectra of substances software. Asian Journal of Pharmaceutical and Clinical Research, 48-56.

[7]. Filimonov, D., Lagunin, A., Gloriozova, T., Rudik, A., Druzhilovskii, D., Pogodin, P., & Poroikov, V. (2014). Prediction of the Biological Activity Spectra of Organic Compounds Using the Pass Online Web Resource. Chemistry Of Heterocyclic Compounds, 50, 444-457.

[8]. Jairajpuri, D., Hussain, A., Nasreen, K., Mohammad, T., Anjum, F., & Tabish Rehman, M. et al. (2021). Identification of natural compounds as potent inhibitors of SARS- CoV-2 main protease using combined docking and molecular dynamics simulations. Saudi Journal Of Biological Sciences, 28, 2423-2431

[9]. Muhammad Torequl Islama, Eunüs S. Ali, Shaikh J. Uddin, Subrata Shaw, Md Amirul Islam, Md Iqbal Ahmed, Manik Chandra Shill, Utpal Kumar Karmakar, Nagendra Sastry Yarla, Ishaq N. Khan, Md Morsaline Billah, Magdalena D. Pieczynska, Gokhan Neagoen, Apostol Apostolov, Maciej Banachr, Andy W.K. Yeung, Amr El-Demerdash, Jianbo Xiao, Prasanta Dey, Santosh Yele, Artur Jóźwik , Nina Strzałkowska, Joanna Marchewka, Kannan R.R. Rengasamya, Jarosław Horbańczuk, Mohammad Amjad Kamal, Mohammad S. Mubaraka, Siddhartha K. Mishra, Jamil A. Shilpi, Atanas G. Atanasov . (2018). Phytol: A review of biomedical activities. Food and Chemical Toxicology , 121, 82-94.

[10]. Alexandra M.S. Carvalho, Luana Hemifarth, Erik Willyame Menezes Periera, Fabricio Santana Oliveira, Irwin R.A. Menezes, Henrique D.M. Coutinho, Laurent Picot, Angello Roberto Antoniolli , Julliyana S.S.Quintans, Lucindo J. Quintans-Junior. (2020). Phytol, a Chlorophyll Component, Produces Antihyperalgesic, Antiinflammatory, and Antiarthritic Effects: Possible NFκB Pathway Involvement and Reduced Levels of the Proinflammatory Cytokines TNF-α and IL-6. Journal of natural products , 83, 1107-1117.

[11]. Josue de Moraes, Rosimeire N. de Oliveira, Jessica P. Costa, Antonio L. G. Junior, Damia ˜o P. de Sousa, Rivelilson M. Freitas, Silmara M. Allegretti, Pedro L.S. Pinto. (2014). Phytol, a Diterpene Alcohol from Chlorophyll, as a Drug against Neglected Tropical Disease Schistosomiasis Mansoni. Plos Neglected Tropical Diseases , 8, 1-12.

[12]. Vasudevan Aparna, Kalarickal V. Dileep, Pradeep K. Mandal, Ponnuraj Karthe, Chittalakkottu Sadasivan, Madathilkovilakathu Haridas. (2012). Anti-Inflammatory Property of n-Hexadecanoic Acid: Structural Evidence and Kinetic Assessment. Chemical Biology and Drug design , 80, 434-439.

[13]. Eric Boilard, Ying Lai, Katharine Larabee, Barbara Balastreiri, Farideh Ghomashchi, Daisuke Fujioka, Reuben Gobeezie, Jonathan S. Coblyn, Michael N. Weinblatt, Elana M. Massarotti, Thomas S. Thornil, Maziar Divangahi, Heinz Remold, Gerard Lambeau, Michael H.Gelb, Jonathan P. Arm, David M. Lee. (2020). A novel anti-inflammatory role for secretory phospholipase A2 in immune complex mediated arthritis. EMBO molecular modicine , 2, 172-187.

[14]. G. Agoramoorthy, M. Chandrasekaran, V. Venkatesalu, M.J. Hsu. (2007). Antibacterial And Antifungal Activities Of Fatty Acid Methyl Esters Of The Blind-Your-Eye Mangrove From India. Brazilian Journal of Microbiology , 38, 739-742.

[15]. Camila Carolinade Menezes Patrício Santos, Mirian Stiebbe Salvadori, Vanine Gomes Mota, Luciana Muratori Costa, Antonia Amanda Cardosode Almeida, Guilherme Antônio Lopesde Oliveira, Jéssica Pereira Costa, Damião Pergentino de Sousa, and Antioxidant Activities of Phytol In Vivo and In Vitro Models. Neuroscience Journal , 1-9.3

[16]. Raman B, V., LA, S., M, P., Rao, N., Krishna, N., M, S., & TM, S. (2012). antibacterial, antioxidant activity and GC-MS analysis of Eupatorium

odoratum. Asian Journal Of Pharmaceutical And Clinical Research, 99-106

[17]. Deeba Shamim Jairajpuri, Afzal Hussain, Khalida Nasreen, Taj Mohammad, Farah Anjum, Md. Tabish Rehman, Gulam Mustafa Hasan, Mohamed F. Alajmi, Md. Imtaiyaz Hassan. (2021). 190 Identification of natural compounds as potent inhibitors of SARS-CoV-2 main protease using combined docking and molecular dynamics simulations. Saudi Journal of Biological Sciences , 28, 2423-2431.

[18]. Camila Carolinade Menezes Patrício Santos, Mirian Stiebbe Salvadori, Vanine Gomes Mota, Luciana Muratori Costa, Antonia Amanda Cardosode Almeida, Guilherme Antônio Lopesde Oliveira, Jéssica Pereira Costa, Damião Pergentino de Sousa, Rivelilson Mendes de Freitas, Reinaldo Nóbrega de Almeida . (2013). Antinociceptive and Antioxidant Activities of Phytol In Vivo and In Vitro Models. Neuroscience Journal , 1-9

[19]. Mohammad Taghi Ghaneian, Mohammad Hassan Ehrampoush, Ali Jebali, Seyedhossein Hekmatimoghaddam, Mohammad Mahmoudi. (2015). Antimicrobial activity, toxicity and stability of phytol as a novel surface disinfectant. Environmental Health Engineering and Management Journal , 2, 13-16.

[20]. Rajasekhar Chikati , Santhi Latha Pandrangi, Ravikumar Gundampati, Harika Sai Vemuri, Meena Lakhanpal, Surya S. Singh, Sunita Saxena, Chitta Suresh Kumar. (2018). Molecular Studies on Evaluation of Phytol as Cytoskeleton Targeting Element in Cancer. International journal of Science & Engineering Research , 9, 1978-1992

[21]. Hamedi, A., Mohagheghzadeh, A., & Rivaz, S. (2013). Preliminary pharmacognostic evaluation and volatile constituent analysis of spathe of Phoenix dactylifera L. (Tarooneh). Pharmacognosy Journal, 5, 83-86.

[22]. Obode, O., Adebayo, A., & Li, C. (2020). Gas chromatography-mass spectrometry analysis and in vitro inhibitory effects of Phoenix dactylifera L. on key enzymes implicated in hypertension. Journal Of Pharmacy & Pharmacognosy Research, 475-490

[23]. Phylip, L., Lees, W., Brownsey, B., Bur, D., Dunn, B., & Winther, J. et al. (2001). The Potency and Specificity of the Interaction between the IA3 Inhibitor and Its Target 276(3), 2023-2030.

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