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Research Article

Isolated Burn Skin Pathogens: Screening Against Extract of Carissa Edulis Vahl and Computational Studies

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ABSTRACT

The extract of Carissa edulis Vahl was evaluated for the potential therapeutic effects against pathogens isolated from the skin of burn patients such as Pseudomonas aeruginosa, Staphylococcus aureus, acinetobacter baumannii, Klebsiella spp, Proteus vulgaris and Escherichia coli. The biological screening results exhibited that methanol extract has more potential therapeutic effect than n-hexane extract. Considerable zone of inhibition was observed for both the extract against *S. aureus* and E. coli. The computational studies were carried out for all components to calculate physicochemical parameters and drug likeness and portrayed that all components found in compliance with the Lipinski rule of five and have the bioactivity score in the category of active drugs.

Keywords: Carissa edulis Vahl extraction, burn skin pathogens, drug likeness and physicochemical property.

INTRODUCTION

Currently the dermatophytres are usually treated by the commercially available antifungal agents in spite of their side effects and cell toxicity. The cell cell toxicity and the side effects by the available therapeutic agents prompting researchers to establish a novel approach employing the plant materials. Exploring the unexplored aspect of the plants for developing antidermatophytic drugs is a novel attempt which needs further investigation. There are 250 genera and 200 species belong to Apocyanaceae family and genus Carissa is among the seven genera found in Saudi arabia[1-5]. The genus is well reported to possess the components such as cardiac glycosides, sesquiterpenes, flavonoids, phenolic compounds, lignans, chlorogenic acid derivatives[6-9], Generally, *C. edulis* is applied to treat headache, chest complains, rheumatism, oedema, gonorrhoea, syphilis, rabies and it is also used as a remedy for fever, sickle cell anaemia, cough, ulcer, toothache, and worm infestation[6-9]. Variety of research has been carried out to evaluate the drug likeness and physicochemical properties for better understanding with respect to the potential antiomicrobial efficacy of the components present in plat extract[10-11]. In a variety of studies *C. edulis* has been found to act as potential antiviral, anticonvulsant, antiplasmodial, antimicrobial, analgesic diuretic as well as hypoglycaemic activity[9,12-16]. Recently the root bark extract of C. edulis has been investigated as an anticonvulsant agent[17]. In recent study the ethanol extract of *C. edulis* Vahl. root bark was evaluated for antimicrobial and cytotoxicity studies[18]. Some other studies also represented the importance of *C. edulis* extract[19-23]. In search of some new potential therapeutic antimicrobial agents, our study targeted the extraction of *C. edulis* and screening against the isolated burn skin pathogens and computational studies.

MATERIALS AND METHOD

Extraction and phytochemical screening

Aerial parts of *C. edulis* Vahl obtained from Aqubat Tanouma Baljorashi, southern region of Saudi Arabia, were dried, powdered and were extracted using the solvents methanol and n-hexane[6]. The phytochemical screening of the plant extract portrayed the presence of components 1-8 shown in the figure-1.

Antimicrobial screening

The isolated, identified and biochemically characterized pathogens: *Pseudomonas aeruginosa, Staphylococcus aureus, acinetobacter baumannii, Klebsiella spp, Proteus vulgaris* and *Escherichia coli* were sub-cultured in nutrient agar medium and incubated for 18 h at 37 ^{0}C, using

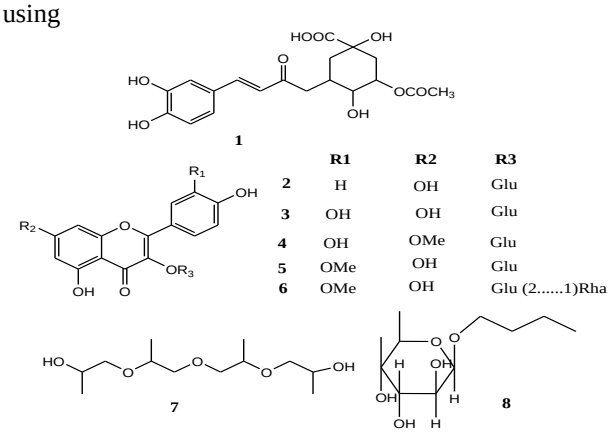

Figure 1: Exhibiting the structures of components present in the *C. edulis* Vahl extract 1-8

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Table 1: Representing the zone of inhibition of the methanol extract of *C. edulis* Vahl, against the isolated pathogens from burn patient.

Pathogens	Effect of n-hexane extract on Microorganism				
	50 µg/ml	25 µg/ml	12.5 µg/ml	6.25 µg/ml	3.125 µg/ml
P. aurigenosa	18.32±0.14	14.22±0.42	10.14±0.22	-	-
S. aureus	20.12±0.22	17.04±0.32	14.72±0.22	12.30±0.08	10.10±0.12
P. vulgaris	13.16±0.12	10.14±0.10	-	-	-
E. coli	21.23±0.15	18.23±0.10	17.14±0.12	15.25±0.20	12.24±0.16
Klebsiella spp.	19.12±0.06	16.72±0.32	13.27±0.10	10.40±0.17	-
A. baumannii	17.32±0.08	14.76±0.14	10.37±0.14	-	-

Table 2: Representing the zone of inhibition the n-hexane extract of *C. edulis* Vahl, against the isolated pathogens from burn patient

Pathogens	Effect of methanol extract on Microorganism				
	50 µg/ml	25 µg/ml	12.5 µg/ml	6.25 µg/ml	3.125 µg/ml
P. aurigenosa	14.32±0.12	12.16±0.18	10.32±0.22	-	-
S. aureus	15.16±0.31	13.12±0.10	10.72±0.12	-	-
P. vulgaris	11.23±0.12	-	-	-	-
E. coli	17.15±0.39	14.18±0.21	10.33±0.10	-	-
Klebsiella spp.	15.32±0.41	10.14±0.08	-	-	-
A. baumannii	14.34±0.14	10.21±0.34	-	-	-

Table 3: Representing the zone of inhibition of the standard, methanol and hexane, against the isolated pathogens from burn patient.

Microorganism			
	Ciprofloxacin (10 µg/ml)	Methanol	Hexane
P. aurigenosa	34.24 ±0.31	-	-
S. aureus	21.46 ±.31	-	-
P. vulgaris	24.56±0.27	-	-
E. coli	23.82±0.47	-	-
Klebsiella spp.	21.34±0.42	-	-
A. baumannii	18.76±0.30	-	-

Ciprofloxacin as positive control and hexane and methanol as negative control[26-29].

Physicochemical properties and bioactivity score

All the parameters for physicochemical properties and bioactivity score were checked with the help of software Molinspiration drug-likeness score online (www. molinspiration.com)[29-32].

RESULTS AND DISCUSSION

Antimicrobial screening

The results of antimicrobial evaluation against all the burn skin pathogens were portrayed that methanol extract has more antimicrobial potential than the n-hexane, the detailed results are provided in the table-1, 2 & 3. From the results it can also be observed that the methanol extract of *C. edulis* Vahl found more active against *S. aureus* and *E. Coli* up to 3.125 µg/ml, while against *P. aurigenosa* and *A. Baumannii*, the effect is observed only up to 12.5 µg/ml. On the other hand the antimicrobial effects against all pathogens, studied were found limited to the concentration up to 12.5 µg/ml, after this concentration no effect was observed.

Physicochemical properties & bioactivity score

Physicochemical parameters & drug likeness were calculated employing the above protocol and results exhibited that all the components of *C. edulis* Vahl are in compliance with the Lipinski rule of five and also have the bioactivity score in the category of active drugs. Lipinski rule o five state's that for an active drug the parameters such as molecular weight, hydrogen bond donors, hydrogen bond acceptors, partition coefficient and number of violation should be within 500, 5, 10, 5 and 4 correspondingly. The properties studied described molecular flexibility, permeability and chance for binding to the receptor. On the other hand for an active drug the bioactivity score is more than 0.00 then it is active, if -0.50 to 0.00 then moderately active, if less than -0.50 then inactive. The calculated bioactivity score portrayed that the bioactivity score for all the component is lying under the category of active drugs, table-4,5.

CONCLUSION

The aerial parts of *C. edulis* Vahl was extracted and screened against the isolated burn skin pathogens. The results for screening against burn skin pathogens explained that the methanol extract has more potential therapeutic effect than the hexane portion. The components of the plants obtained by phytochemical screening were subjected for calculation of molecular properties such as drug likeness and physicochemical properties. The computational studies showed that all the components are following the Lipinski rule of five and have significant bioactivity score corresponding to the zone for active drug. The designed approach to analyse the antimicrobial activity of *C. edulis* extract and the calculation of molecular properties described that it can be used as the future antimicrobial agent will also help researcher for further research and development.

CONFLICT OF INTEREST

Table 4: Representing the physicochemical properties of all the components of *C. edulis* Vahl extract.

Physicochemical property score	Components								
	1	2	3	4	5	6	7	8	Standard
miLogP	-0.45	0.12	-0.36	2.22	1.99	1.99	0.45	0.43	-0.701
TPSA	164.74	190.28	210.50	120.36	120.36	120.36	68.16	79.15	74.569
Natoms	25	32	33	23	23	23	17	16	24.0
MW	354.31	448.38	464.38	316.26	316.26	316.26	250.34	234.29	331.347
nON	9	11	12	7	7	7	5	5	6
nOHNH	6	7	8	4	4	4	2	3	2
Nviolations	1	2	2	0	0	0	0	0	0
Nrotb	5	4	4	2	2	2	10	4	3
Volume	296.27	364.19	372.21	257.61	257.61	257.61	256.39	227.72	285.46

Table 5: Representing the bioactivity score of all the components of *C. edulis* Vahl extract.

Bioactivity score	Components								
	1	2	3	4	5	6	7	8	Reference
GPCR ligand	0.29	0.05	0.06	-0.11	-0.10	-0.10	-0.32	0.03	0.12
Ion channel modulator	0.14	-0.05	-0.04	-0.27	-0.26	-0.26	-0.17	0.20	-0.04
Kinase inhibitor	-0.00	0.10	0.13	0.21	0.25	0.25	-0.30	-0.35	-0.07
Nuclear receptor ligand	0.74	0.20	0.20	0.27	0.28	0.28	-0.31	-0.02	-0.19
Protease inhibitor	0.27	-0.05	-0.06	-0.27	-0.30	-0.30	-0.36	0.04	-0.21
Enzyme inhibitor	0.62	0.41	0.42	0.20	0.22	0.22	0.02	0.66	0.28

The authors have no conflict of interests

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REFERENCES

1. Rahman M. A, Al-Said M S., Mossa J S., Al Yahya M A, Al Hemaid M A F. A check List of Angiosperm Flora of Farasan Islands, Kingdom of Saudi Arabia. Pakistan Journal of Biological Sciences 2002; 5(11): 1162-1166.
2. Rahman, M A, Mossa, J.S. Al-Said, M.S, Al-Yahya, M.A. Medicinal plant diversity in the flora of Saudi Arabia 1: a report on seven plant families. Fitoterapia 2004; 75(2): 149-161.
3. Burkill, H.M. The Useful Plants of West Africa, 2nd Ed vol. I. Families A-D Royal Botanical Gardens. Kew. 1985, 145-146.
4. Hutchinson, J.; Dalziel, J. M. Flora of West Africa, vol. II Crown Agents for Over sea Governments and Administration, Milbank, London S.W.I. 1963, 51-54.
5. Irvine, F.R., Woody Plants of Ghana. Oxford University Press, London. 1961, 616–618.
6. Al-yuossef, H.M., Hassan, W.H., Chemical constituents of *Carissa edulis* Vahl, Biosci. Biotechnol. Res. Asia 2010; 7: 635–646.
7. El-Youssef H.M., Murphya B.T., Amer M.E., AbdelKader M.S., Kingston D.J. I. Phytochemical and Biological Study of the Aerial Parts of Lotus Lalambensis Growing in Saudi Arabia. Saudi Pharmaceutical Journal 2008; 16 (2): 122-134.
8. Kirira, P.G., Rukungo, G.M., Wanyonyi, A.W. Anti-plasmodial activity and toxicity of extracts of plants used in traditional malaria therapy in Meru and Kilifi Districts of Kenya. J. Ethnopharmacol. 2006; 106: 403-407.
9. Pal, D.R., Kulshreshtha, R.P., Rastoqi, A. A new lignan from Carissa carandas. Phytochemistry 1975; 14: 2302-2303.
10. Alodeani E A, Arshad M, Izhari M A. Drug likeness and physicochemical properties evaluation of the alkaloids found in black pepper: piperine, piperidi ne, piperettine and piperanine. European Journal of Pharma and medical research 2015; 2(6): 296-301.
11. Alodeani E A, Arshad M, Izhari M A. Antileishmanial screening, physicochemical properties and drug likeness of pyrazole carbaldehyde derivatives. Asian Pac. J. Health Sci. 2015; 2(2): 41-47.
12. Achenbach, H., Weibal, R and Addae-Mensah, I. Lignan from Carissa edulis. Phytochemistry. In Biological Abstract 1983; Vol. 76(5): 30837-38545.
13. Bentley, M. D., Brackett, S. R. and Chapya, A. 2-Hydroxyacetophenone, Principal Root Volatile of the East African Medicinal Plant, Carissa edulis. Journal of Natural Products 1984; (47): 1056-1057.
14. Tolo, F.M., Rukungo, G.M., Muli, F.W. Anti-viral activity of the extracts of a Kenyan medicinal plant Carissa edulis against herpes simplex virus. J. Ethnopharmacol 2006; 104, 92-99.
15. Ya'u Yaro, A.H., Abubakar, M.S., Hussaini, I.M., J. Anticonvulsant activity of. Carissa edulis (Vahl) (Apocynaceae) root bark extract. Ethnopharmacol. 2008;120: 255-258.
16. *Jawaid T., Argal S., Singh S.*, Botanicals and herbs: A traditional approach in treatment of epilepsy. *J. Pharm. Res. 2011*; *4*(*4*):*1138-1140*.
17. Yaro A.H., Abubakar M.S., Anuka J.A., Hussaini I.M. Anticonvulsant activity of Carissa edulis (Vahl) (Apocynaceae) root bark extract. Journal of Ethnopharmacology 2008; 120: 255-258.

18. Ibrahim H, Ngulde S, Kyari Sandabe U, Bashir Tijjani M, Alkali Barkindo A, Marte Hussaini I. Phytochemical constituents, antimicrobial screening and acute toxicity studies of the ethanol extract of Carissa edulis Vahl. root bark in rats and mice. American Journal of Research Communication 2013; 1(9).
19. Ibrahim, H. Pharmacognostic and Biological (Analgesic Activity) Studies of Carissa edulis Vahl. Ph. D. Thesis. Ahmadu Bello University, Zaria, Nigeria 1997; 232.
20. Tolo F M., Rukunga G M., Muli F W., Ochora J, Eizuru Y, Muthaurn C N., Kimani C W., Mungai G M, Kofi M W. In vitro anti-viral activity of aqueous extracts of Kenyan Carissa edulis Prunus africana and Melia azedarach against human cytomegalovirus. African Journal of Health Sciences 2007;14.
21. Gitahi S. M, Juma K. K, Mwangi B. M, Njagi J. M, Mworia J. K, Aliyu U, Mwonjoria K. J, Njoroge W. A, Mburu N. D, Ngugi M. P. Antinociceptive properties of dichloromethane: methanolic leaf and root bark extracts of Carissa edulis in rats. The Journal of Phytopharmacology 2015; 4(2):106-112.
22. Yilangai M.R., Chaskda A. A., Mwansat G. S., Akwashiki. O. A comparison of insect fruit utilization of Carissa (Carissa edulis Vahl) and Jasmine (Jasminum dichotomumVahl) in a protected habitat. IOSR Journal of Environmental Science, Toxicology and Food Technology 2013; 7 (1): 43-47.
23. Okullo J.B.L, Omujal F., Bigirimana C., Isubikalu P., Malinga M., Bizuru E., Namutebi A., Obaa B.B., Agea J.G. Ethno-Medicinal Uses of Selected Indigenous Fruit Trees from the Lake Victoria Basin Districts in Uganda. Journal of Medicinal Plants Studies2014 ; 2 (1): 78-88.
24. Xin Li, Shutao MA. Advances in the discovery of novel antimicrobials targeting the assembly of bacterial cell division protein FtsZ. European Journal of Medicinal Chemistry 2015; 95 (5): 1-15.
25. Alodeani E A, Arshad M, Izhari M A. Burn skin pathogens: Isolation, identification and antimicrobial activity pattern against pyrazole derivatives. American Journal of Pharm Tech research 2015, 5(6): 150-158.
26. Iram N, Khan M S, J Reshma, Arshad M, Alam M, Alam P, Khan R H, Firdaus F: Interaction mode of polycarbazole-titanium dioxide nanocomposite with DNA: Molecular docking simulation and in-vitro antimicrobial study. Journal of Photochemistry and Photobiology B: Biology 2015; 153: 20-32.
27. Bushra R, Shahadat M, Khan M A, A R., Arshad M, Rafatullah M, Naushad M: Preperation of Polyaniline based Nanocomposite material and their Environmental Applications. Int. J. Env. Sci. Technol. 2015.
28. Alodeani E A, Arshad M, Izhari M A. Anti-uropathogenic activity, drug likeness, physicochemical and molecular docking assessment of (E-)-N' -(substitutedbenzylidene)-2-(quinolin-8-yloxy) acetohydrazide. Asian Pac J Trop Biomed 2015; 5(8): 676–683.
29. Nova ulica. Molinspiration cheminformatics [homepage on the internet], SK-900 26 Slovensky Grob, Slovak Republic [cited 2012 July3], Available from http://www.molinspiration.com.
30. Verma, A. Lead finding from Phyllanthus debelis with hepatoprotective potentials Asian Pacific Journal of Tropical Biomedicine 2012; S1735-S1737.
31. Lipinski CA, Lombardo F, Dominy BW, Feeney PJ. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. Adv. Drug Delivery Rev. 1997; 23(1-3): 3-25.
32. Alodeani E A, Arshad M, Izhari M A. Antileishmanial screening, physicochemical properties and drug likeness of pyrazole carbaldehyde derivatives: Asian Pac. J. Health Sci. 2015; 2(2): 41-47.