

Drugs Candidate's Interactions with the Main Protease Enzyme (Mpro) of Covid-19 by Molecular Docking Studies

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Abstract

Background and objective: A critical antiviral target is the SARS-CoV-2 main protease (Mpro), and our aim was to identify drug compounds as inhibitors of Covid-19 protease using molecular docking and to evaluate their ability to interaction with main protease(Mpro).

Materials and methods: The main protease structure of Covid-19 (Mpro) with code 6M03 and the structure of 64 drug compounds were obtained from PDB and Chem Spider. Molecular docking was performed with Auto Dock Vina software. The results were analyzed by Biovia Discovery Studio 4.5.

Results: Cidofovir, Emtricitabine, Ganciclovir, Lamivudine, N4-Hydroxycytidine, Tenofovir, Vidarabine, L-Pyroglutamic acid and Tyr -His-Asn with ΔG -4.5 to -6.6 kcal / mol , are in the active site.

Conclusion: the ligands are negatively bound to the target protein; it makes equal importance to all of these protease inhibitory ligands. However, the best binding energy value of -6.6 kcal / mol was obtained for the tri peptide Tyr-His-Asn.. It seems that this tri -peptide should be considered in in-vitro and in-vivo study. Molecular docking studies also showed that this protease did not bind to Remdesivir at the active site.

Keywords: Covid-19, Protease (Mpro), Molecular Docking, AutoDock, AutoDock Vina

Effectiveness of Hand Sanitizers against Human Microbiota of the Skin during the COVID-19 Pandemic

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Abstract

Control of COVID-19 and its pandemic has become a health crisis in the world. Due to the high latency period of this virus and its transmission, we are facing with the overwhelming prevalence of this disease. However, it is possible to prevent the spread of the virus using the implementing control strategies and management of effective hygiene procedures. Skin is the largest organ of the human body and is known as the first defense against the microbial pathogens, on the other hand, skin is an appropriate habitat for diverse and complex collection of bacteria. Hands are important risk factors for the spread of the infection, and the use of hand sanitizers reduces the number of skin microbiota which results in many different allergic reactions and also increases the bacterial resistance against different antimicrobial agents. Also, they may increase the risk of skin cancer. This review has focused on the effectiveness of hand hygiene on the diversity of skin microbiota during the COVID-19 pandemic, and also the importance of surface disinfectants in reducing or disrupting of infection transmission. In addition, the antibacterial mechanisms of different disinfectants and their effects on the transmission of Covid-19 will be discussed.

Key words: COVID-19, hand microbiota, disinfectants

Frequency of Genes Encoding Toxic Shock Syndrome and Exfoliative Toxins among Methicillin Resistant *Staphylococcus aureus* Strains Isolated from Patients in Isfahan. 2017-19

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Abstract

Background and objective: *Staphylococcus aureus* produces a wide variety of exoproteins that contribute to its ability to colonize and cause disease in mammalian hosts. Nearly all strains secrete a group of enzymes and cytotoxins and some strains produce one or more additional exoproteins, which include toxic shock syndrome toxin-1 (TSST-1), the staphylococcal enterotoxins, the exfoliative toxins (ETA and ETB), and leukocidin. The aim of this study was to determine the frequency of *tsst*, *eta*, and *etb* genes encoding TSST-1, ETA and ETB, respectively, among methicillin resistant *S. aureus* (MRSA) strains isolated from 2 referral hospitals in Isfahan.

Material and methods: During 2017 and 2019 a total of 307 MRSA strains were collected from patients in 2 referral hospitals in Isfahan. All isolates were identified using specific primers for *nucA* and *mecA* genes. For typing of bacterial strains, prophage typing using multiplex-PCR was employed and presence of *tsst*, *eta* and *etb* genes was determined using separate PCR assays.

Results: Using PCR by specific primers all bacterial isolates were confirmed as MRSA. Six prophage types SGA (6%), SGB (63%), SGF (100%), SGFa (100%), SGFb (100%) and SGL (6%) and also 4 prophage patterns were identified among strains, in which pattern 3 was the dominant one. Moreover, 63% of strains were positive for both *tsst* and *eta* genes and *etb* gene was not detected among the strains.

Conclusion: The results of the present study indicated the high prevalence of MRSA strains harbored genes encoding TSST-1 and exfoliative toxin in studied hospitals in Isfahan.

Keywords: *S. aureus*, methicillin, prophage typing, TSST-1, exfoliative toxin, multiplex-PCR

Antimicrobial Activity of Aqueous and Ethanolic Extracts of Leaves of Walnut against Some Pathogenic Bacteria: A Laboratory Study

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Abstract

Background and objective: Walnut is a rich source of health-promoting flavonoids and phenolics with antimicrobial properties. The aim of this study was to evaluate the *in-vitro* antimicrobial effect of aqueous and ethanolic extracts of walnut leaf on *Escherichia coli*, *Salmonella typhi*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, and *Listeria innocua*.

Materials and methods: Aqueous and ethanolic extract of walnut leaf were extracted by maceration method. The antimicrobial activity was evaluated through pour plate, disk diffusion agar, well diffusion agar, minimum inhibitory concentration (MIC), and minimum bactericidal concentration (MBC). Data were analyzed by SPSS software and Duncan test ($p < 0.05$).

Results: All the bacterial species were sensitive to the extract. In disk and well diffusion agar methods, *S. aureus* was the most sensitive bacteria to the aqueous and ethanolic extracts. The MIC of the aqueous extract of walnut leaf for *Escherichia coli*, *Salmonella typhi*, *Pseudomonas aeruginosa*, *Staphylococcus aureus* and *Listeria innocua* was 50, 50, 25, 12.5 and 25 mg/ml, respectively. The MIC of the ethanolic extract of walnut leaf for *Escherichia coli*, *Salmonella typhi*, *Pseudomonas aeruginosa*, *Staphylococcus aureus* and *Listeria innocua* was 50, 50, 25, 12.5 and 12.5 mg/ml, respectively. For all bacteria the MBC of aqueous and ethanolic extracts of walnut leaf was larger than the MIC.

Conclusion: The antimicrobial effect of the ethanolic extract was higher than the aqueous extract, and gram-positive bacteria were more sensitive to the extract compared to the gram-negative ones. The aqueous/ethanolic extract of walnut leaf could be used as a natural antimicrobial.

Keywords: Walnut leaf, Aqueous extract, Ethanolic extract, Antimicrobial activity

Larvicidal Effect of Spearmint (*Mentha spicata*) and Rosemary (*Rosmarinus officinalis*) against Larvae of *Culex*

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Abstract

Background and objective: Mosquitoes are vectors or intermediate hosts for several infectious microorganisms worldwide. Due to harmful effects on the environment, high operating costs, as well as the resistance of mosquitoes to chemical insecticides, the need for biological control of mosquitoes has been considered by researchers. In the present study, the larvicidal effect of essential oil of spearmint (*Mentha spicata*) and rosemary (*Rosmarinus officinalis*) against larvae of *Culex* was investigated.

Materials and methods: From May to September 2018 a total of 1,200 larvae of *Culex* mosquitoes were caught from four areas of Qarachai river located in Khondab city of Markazi province. The larvae were encountered to concentrations of 10, 50, 200 and 600 ppm aqueous solution of spearmint and rosemary essential oils produced by Barij Essence Pharmaceutical Company. Larval mortality was assessed at 6, 12, 24, 48 and 72 hours after exposure to the tested materials. The experiment was repeated three times and for each concentration, the average number of killed larvae was calculated. For negative control distilled water and for positive control 1 ppm cocentration of organophosphate larvicide “Temephose” were prepared and tested.

Results: Although all concentrations of spearmint and rosemary essential oils at different timepoints showed some degree of effect on the larvaa, spearmint essential oil at 200 ppm and at 6 hours, showed the fastest and highest larvical effect.

Conclusion: The present study showed that both essential oils, especially spearmint, could be considered as a potential alternative to chemical insecticides for biological control of *Culex* mosquito larvae.

Keywords: essential oil, spearmint, rosemary, larvicidal effect, mosquito

Antioxidant Power and Antimicrobial Activity of Hydro-alcoholic Extract of *Echinacea purpurea* on *Escherichia coli*, *Salmonella typhi*, *Staphylococcus aureus* and *Bacillus cereus*

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Abstract

Background and objective: The increased resistance of bacteria to antibiotics has increased the tendency of consumers to use natural antimicrobial compounds. *Purple Coneflower* (*Echinacea purpurea*) contains bioactive compounds and it has long been used to treat many diseases. The aim of this study was to investigate the total content of phenolics and flavonoids, antioxidant activity, and antimicrobial property of hydro-alcoholic extract of *Purple Coneflower* on some pathogenic microorganisms.

Materials and methods: In this study, the hydro-alcoholic extract (50% distilled water + 50% ethanol) was prepared according to the maceration method. Total content of phenolics and flavonoids, and antioxidant activity (DPPH and ABTS radical scavenging) were determined. The antimicrobial activity was evaluated through disk diffusion agar, well diffusion agar, minimum inhibitory concentration, and minimum bactericidal concentration, against *Escherichia coli*, *Salmonella typhi*, *Staphylococcus aureus*, and *Bacillus cereus*.

Results: The minimum bactericidal concentrations for *S. aureus*, *B. cereus*, *E. coli*, and *S. typhi* were 16, 32, 64, and 64 mg/ml, respectively. In disk and well diffusion agar methods, the lowest and highest inhibition zones were observed for *S. typhi* and *S. aureus*, respectively. The hydro-alcoholic extract had a remarkable level of phenolic and flavonoid compounds and antioxidant activity.

Conclusion: The hydro-alcoholic extract of *Purple Coneflower* had a considerable antimicrobial effect against the bacterial species tested; however, the gram-positive bacteria were more sensitive to the extract in comparison to the gram-negative ones. Therefore, the *Purple Coneflower* could be used as an effective antimicrobial agent against pathogenic microorganisms.

Keywords: Purple Coneflower, Hydro-alcoholic extract, Pathogenic bacteria, Antimicrobial