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Formulation and Physicochemical Characterization of Stable Gel Containing *Ziziphus Jujuba* Fruit Extract

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17-20 February 2021

Poster 1

Abstract Presenter:

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Introduction: Utilizing herbal medicine since the era of ancient civilizations has proven the importance of natural therapeutic formulations in skin care. *Ziziphus Jujube*, which grows in various parts of its natural habitat in Iran, has been used for centuries in herbal medicine for treatment of a variety of ailments. The various effects of jujube fruit extract are due to the presence of various compounds such as flavonoids, phenolic acids, terpenes, alkaloids and polysaccharides. *Ziziphus Jujube* extract has shown anti-inflammatory and anti-oxidant properties on skin. Up to yet there was not any skin products of this extract available in the Iranian and world markets. Hence, it is necessary to conduct a study on formulating and physicochemical evaluation of *Ziziphus Jujube* fruit extract The present research was undertaken with the aim to formulate and evaluate a topical anti-oxidant gel containing *Ziziphus Jujube* aqueous extract.

Methods and Materials: Fruits of *Ziziphus Jujube* were collected from Birjand, Iran and aqueous extract was obtained by digestion method. The gel formulation was designed using aqueous extract of *Ziziphus Jujube* fruit in 5% w/v concentration and was carried out using various polymer bases (Carbopol 934 and 940). The physiochemical parameters of mentioned formulations such as pH, rheology, spreadability, appearance, etc. were determined. Finally, the chosen formulation was evaluated in determination of phenolic content, release, stability and Free radical scavenging assay tests.

Results: The best results were obtained from the gel prepared with 1.5% Carbopol 934, 5% ethanol, 5% glycerin and 0.03% methyl and propyl paraben with pH=6.3±0.01. The final formulation showed pseudo plastic rheological behavior and the kinetic of release was zero-order. Acceptable results were also obtained from stability and free radical scavenging assay tests and the amount of phenolic content was measured as 33.89±0.017 µg GAE/mg.

Discussion and Conclusion: Based on the physicochemical, stability and free radical scavenging assay tests' results, this formulation of *Ziziphus Jujube* fruit extract could demonstrate the potential for use as a new, safe, beneficial and natural topical anti-oxidant product.

Keywords: topical anti-oxidant, herbal gel formulation, *Ziziphus jujube*, topical gel formulation

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Preparation and Evaluation of a Topical Gel Formulation of *Salvia officinalis* Aerial Branches and *Calendula officinalis* Flowers Extracts

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17-20 February 2021

Poster 2

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Introduction: Utilizing herbal medicine since the era of ancient civilizations has proven the importance of natural therapeutic formulations in skin care. *Salvia officinalis* and *Calendula officinalis* which grows in various parts of their natural habitat in Iran, has been used for centuries in herbal medicine for treatment of a variety of ailments. Skin integrity is a vital issue for maintaining skin ability to protect against water loss, bleeding, and the entry of microorganisms. For this reason, skin protection and improvement of the wound repairing process is really important. Numerous studies have shown the availability of substances such as flavonoids and phenolic acids with antioxidant, antimicrobial, anti-inflammatory and repairing effects in the hydroethanolic extracts of *Calendula officinalis* petals and aerial branches of *Salvia officinalis* which could lead to wound healing effects. According to what is mentioned, topical products containing both of these plants with the ability to repair skin wounds seem beneficial.

Methods and Materials: Plants, were collected through the Tehran market in spring, their hydroethanolic extracts were then obtained by digestion method. The gel formulation was designed using hydroethanolic extracts of *Calendula officinalis* petals in 1% w/v concentration and Salvia officinalis aerial branches in 1% w/v and were carried out using various polymer bases (Carbopol 934 and 940). The physiochemical parameters of mentioned formulations such as pH, rheology, spreadability, appearance, etc. were determined. Finally, the chosen formulation was evaluated in determination of phenolic content, release and stability tests.

Results: The best results were obtained from the gel prepared with 1/5% carbopol 934, 5% glycerin,0/03% methyl paraben, 0/02% propyl paraben and water with pH=6/4±0.01. The final formulation, pseudoplastic rheological behavior, and the kinetic of release was zero-order. Acceptable results were also obtained from stability and the amount of phenolic content was measured as 24/12±0.012 µg GAE/mg.

Discussion and Conclusion: Based on the physicochemical and stability tests this formulation of *Calendula officinalis* and *Salvia officinalis* extracts could demonstrate the potential for use as a safe, beneficial, and natural topical wound healing product.

Keywords: Topical gel formulation, *Calendula officinalis*, *Calendula officinalis*, Carbopol 934, Healing Wounds

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Hollow mesoporous silica nanoparticles for co-delivery of hydrophobic and hydrophilic molecules: mechanism of drug loading and release

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17-20 February 2021

Poster 3

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Introduction: The objective of this study was to investigate the loading capacity and release profiles of curcumin (CUR), as a hydrophobic drug, and doxorubicin hydrochloride (DOX), as a hydrophilic drug, into hollow mesoporous silica nanoparticles (HMSNs).

Methods and Materials: HMSNs were synthesized by a modified Stöber method. The physicochemical properties of the nanoparticles were investigated using different techniques including DLS, Zetasizer, TEM, EDXS, BET, FTIR and TGA. CUR and DOX were loaded in HMSNs in a nanoparticle-to-drug ratio of 1:2. The drug loading and release studies were conducted and analyzed by HPLC-UV.

Results: The hydrodynamic size and zeta potential of HMSNs were 206.8 nm and -28.8 mV respectively. Drug loadings of DOX into HMSN-DOX NPs and HMSN-DOX-CUR NPs were 37.51±2.07% and 18.57±6.22% respectively, and the loading capacities of CUR in HMSN-CUR NPs and HMSN-DOX-CUR NPs were 61.57±2.82% and 43.73±8.3% respectively. The release study of DOX in phosphate buffer saline (PBS, pH=7.4) showed that 10.36±0.7% and 13.06±0.26% of loaded DOX in HMSN-DOX NPs and HMSN-DOX-CUR NPs was released after 24 hrs, respectively; where 92.04±3.89% and 95.53±0.29% of the loaded CUR in HMSN-CUR NPs and HMSN-DOX-CUR NPs were released after 6 hours in albumin 3%, pH=7.4, respectively.

Discussion and Conclusion: The result of this study confirms that HMSNs can be used as a suitable system for targeting the delivery of hydrophilic drugs in cancer therapies thanks to their ability to sustain the drug release. On the other hand, the release study of CUR as a hydrophobic drug model suggests that the considered NPs may NOT be suitable for targeted delivery of such drugs due to the rapid release of compounds in a simulated plasma model. However, these NPs signal a suitable system for intravenous delivery of highly lipophilic drugs.

Keywords: Hollow Mesoporous Silica NPs, Drug Release, Curcumin, Doxorubicin

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Preparation and in vitro characterization of piperine liposomes as an extended release carrier

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17-20 February 2021

Poster 4

Abstract Presenter:

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Introduction: Piperine (1-Piperoylpiperidine), the major bioactive component from Piper longum and *Piper nigrum*, is an alkaloid with many biomedical applications (1). It has gained increasing attention for its pharmacological effects such as anti-inflammatory, antioxidant, and antibacterial activity (2). However, its low aqueous solubility and bioavailability is considered as the main barrier to its utilization in clinical applications (3). The aim of the present article is to incorporate piperine into liposome as an effective sustained release drug delivery system to overcome these limitations and improve piperine pharmaceutical properties for oral drug delivery.

Methods and Materials: Liposomes of piperine were prepared using thin-film hydration method, which is a common technique to prepare liposomes. The effect of two main formulation factors, including the ratio of cholesterol (Chol) to soybean phosphatidylcholine (SPC) (selected as 10:90 and 40:60) and the ratio of lipid to drug (selected as 10 and 30) on the properties of formulations (size, encapsulation efficiency, and drug release) was determined. Liposomal formulations of piperine were characterized regarding size, encapsulation efficiency, morphology, and drug release profile.

Results: It is shown that the encapsulation efficiency increased with increasing total lipid concentration from 10 to 30 in the formulations. However, increasing cholesterol percentage from 10 to 40 decreased the drug encapsulation in liposomes from 77 to 57%. The optimized liposome formulation (lipid to drug ration =30, Chol% =10) with encapsulation efficiency of 77% and an average diameter of 2 µm exhibited a sustained release over 5 days at 37 degrees C.

Discussion and Conclusion: Current evidence suggests that the amount of cholesterol and the lipid to drug ratio play critical roles in increasing encapsulation efficiency of piperine liposomes. As compared with the conventional dosage form of piperine, the optimum liposome formulation can improve the sustained release of this alkaloid and could be suggested as a promising carrier for the delivery of piperine for oral applications.

Keywords: Liposome, Piperine, Sustained release, Characterization

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Berberine- phospholipid nano-aggregates: preparation and in vitro characterization

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17-20 February 2021

Poster 5

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Introduction: Berberine (Ber), an isoquinoline alkaloid, gained great interest in recent years according to its different pharmacological actions (1). However, poor gastrointestinal absorption and low oral bioavailability have limited its application for further clinical application (2). Lipid–drug conjugates (LDCs) are drug molecules that have been covalently modified with lipids. LDCs have represented many profits such as improved oral bioavailability, reduced toxicity, and enhanced drug loading into delivery carriers (3).

Methods and Materials: In this study, the Ber–soy phosphatidylcholine complex (Ber-SPC) was prepared by the solvent evaporation method. Ber and soy phosphatidylcholine (SPC) at molar ratios of Ber:SPC 1:2 was dissolved in methanol and dichloromethane at volume ratios of 1:9 respectively and then placed in a round bottom flask, kept under continuous stirring (200 rpm) for 3 hours at 40 °C. The resultant mixture was evaporated under vacuum by using a rotary evaporator at 40 °C. Complex formation was confirmed by Fourier transform infrared spectroscopy (FT-IR), powder X-ray diffraction (XRD), scanning electron microscopy (SEM), solubility, and partition coefficient determination. These amphiphilic conjugates may assemble into the nano-aggregates by adding deionized water to the Ber-SPC complex and preparation of 1 mg/mL solution. The mixture was then subjected to either bath sonication or probe sonication or high-pressure homogenization (HPH). Each sizing technique was continued for either 5, 10, or 15 min. The bath sonication was also continued up to 20 min.

Results: Based on the results, the conjugation of SPC to Ber significantly increased the lipophilicity and changed the properties of drugs. The optimized nano-aggregates of Ber-SPC demonstrated a nanometric particle size of 65.82 ± 0.68 nm (PDI = 0.25 ± 0.01) and 92.35 ± 2.01 nm (PDI = 0.25 ± 0.01) after 10 min probe sonicating and 20 min bath sonicating, respectively.

Discussion and Conclusion: Nanosized Ber–SPC aggregates were successfully prepared and characterized as a promising nanocarrier.

Keywords: Phospholipid, Berberine, Nano-aggregates, Characterization

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Study on the effect of different parameters on the preparation of nanosuspension by milling method

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17-20 February 2021

Poster 6

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Introduction: The present investigation was undertaken to study the effect of different process and formulation parameters on the particle size of repaglinide nanosuspension, a poorly soluble anti-diabetic compound. Milling, as the most common method of nanosuspension preparation, was used in this study. Ball to powder ratio and milling time, as well as type and concentration of stabilizer were considered as different variables in this study.

Methods and Materials: Repaglinide was dispersed in an aqueous solution of various stabilizers (polyvinylpyrrolidone (PVP), hydroxypropyl methylcellulose (HPMC) or poloxamer 188), and milled up to 4 hours using planetary ball mill. Sodium lauryl sulfate (SLS) as a co-stabilizer was used in this process with different concentrations. Obtained nanosuspensions were studied in terms of particle size by measuring Z-average (Z-ave) and polydispersity index (PDI). Zeta potential of selected formulations were also evaluated.

Results: The results revealed that using higher ball to powder ratio resulted in lower drug particle size. Also, milling of the dispersion for 3 to 4 hours was more effective in reducing particle size compared to 2 hours of milling, under the same conditions. According to the results, adding lower percent of SLS in the formulations reduced the zeta potential significantly, which is expected to improve its stability. At the same time, increasing SLS concentration resulted in nanosuspensions with higher Z-ave and PDI values, probably due to the particles aggregation. PVP as a stabilizer, led to the formation of more acceptable nanosuspensions in comparison to HPMC and poloxamer 188. The Z-ave and PDI values of the formulations prepared with various PVP concentrations were in the range of 448-515 nm and 0.31- 0.42, respectively.

Discussion and Conclusion: These results indicate that the selection of appropriate formulation and process parameters has a significant effect on the particle properties and the achievement of the desired nanosuspension.

Keywords: Particle size, mining, Nanosuspension, pvp, Ball to powder ratio, stabilizer

References:

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Cytoprotective Effect of Evolocumab As an Antihyperlipidemic Drug Against H2O2-Induced Oxidative Stress in Human Endothelial Cells

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17-20 February 2021

Poster 7

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Introduction: Recent surveys have shown an association between proprotein convertase subtilisin/kexin type 9 (PCSK9) and oxidative stress. In this investigation, the effect of evolocumab an anti-PCSK9 antibody was assessed against oxidative damage caused by hydrogen peroxide (H2O2) in human umbilical vein endothelial cells (HUVEC).

Methods and Materials: Viability of HUVEC was measured by MTT assay. Hydroperoxides and malondialdehyde (MDA) levels, and ferric reducing antioxidant power (FRAP) were detected spectrophotometrically in HUVEC that pre-treated with evolocumab and, then exposed to H2O2.

Results: Evolocumab significantly prevented the cytotoxicity induced by H2O2 at the concentrations of 5-100 µg/ml. Pre-treatment of HUVEC with evolocumab reduced hydroperoxides and MDA levels and also increased FRAP value in intra- and extra-cellular mediums compared with H2O2 stimulated cells at different concentration ranges.

Discussion and Conclusion: This study displayed anti-oxidative and cytoprotective activities of evolocumab against oxidative damage caused by H2O2 in endothelial cells. Regarding a cross talk between PCSK9 and oxidative responses, additional studies are required to confirm the effect of anti-PCSK9 monoclonal antibodies as the novel helpful therapeutic agents in hyperlipidemia against oxidative stress.

Keywords: Evolocumab, Stress oxidative, Antioxidants, Antihyperlipidemia

Reference:

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Monosodium glutamate influences depressive behavior of young and adult mice in forced swimming test: vitamin B6 as a new update remedies the situation

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17-20 February 2021

Poster 8

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Introduction: Depression is a common medical condition that could have severe and chronic outcomes. This ailment may cause serious social damages and increase morbidity and mortality. Glutamate and GABA are two of the main excitatory and inhibitory neurotransmitters, respectively. Change in glutamate, GABA ratio is related with depression. Monosodium glutamate (MSG) could cause metabolic and neurotransmitters disturbance (1). Vitamin B6 is a cofactor for various enzymes (such as glutamate decarboxylase, GAD) and can alter neurotransmitter levels (2). GAD is responsible for converting glutamate to GABA, and following a reduction in the enzyme efficacy the balance between the two neurotransmitters is altered. The aim was observing the effects of MSG administration alone and in combination with vitamin B6 on mood in two age groups of mice.

Methods and Materials: Two age groups of mice were used young (4-5 weeks; 21 g ± 1.5), and adult (9-10 weeks; 29.5 g ± 0.5). Acute or long term MSG was administered alone or in combination with vitamin B6. Total immobility time was measured during the forced swimming test (FST) as an indicator of animal despair. Locomotor test was carried out as a supporting test, before FST.

Results: A single dose of MSG significantly increased immobility time during the FST only in young mice 179 sec ±17 (vs control 159 sec ±8.5). In young and adult animals' immobility time was higher than control on the 7th and 14th days following MSG administration. Vitamin B6 decreased the immobility time during FST in both age groups when it was administered prior to MSG single dose or in combination with MSG for a long term.

Discussion and Conclusion: Therefore, MSG effects on depressive behavior depends on age and duration of exposure. Vitamin B6 would be presented as an update in preventing the harmful effects of MSG on mood possibly by its benefit effects on the neurotransmitter system.

Keywords: vitamin B6, Forced swimming test, Depression, Monosodium glutamat

Reference:

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Comparison of the n-acetylcysteine and n-acetylcysteine niosomes effects on brain tissue in acute paraquat poisoning in male rats

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17-20 February 2021

Poster 9

Abstract Presenter:

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Introduction: Paraquat (PQ) as a bipyridil compound is widely used as an effective herbicide which produces reactive oxygen species (ROS) which can affect the unsaturated lipids of cell membranes leading to cell mortality.
N-acetyl cysteine (NAC) is a medication which has a beneficial role in reducing the intoxication of brain caused by PQ. Niosomes are bilayer vesicles that increase the bioavailability of drugs. The aim of this study, after formulating NAC niosome nanoparticle (NACNP) was to compare the effects of NAC and niosome of NAC (NACNPs) against PQ-induced brain toxicity in relation with its antioxidant activity.

Methods and Materials: In this experimental study 30 male rats weighting from180 to 250 were divided into 5 groups randomly: Control group with normal saline, all following 4 groups poisoned with 35mg/kg/day of PQ intraperitoneal and respectively treated with 25mg/kg/day NAC, 25mg/kg/day noisome and 25 mg/kg/day NACNP by gavage method, respectively.24 hours after last treatment lung homogenate tissue samples were collected from all rats. oxidative stress biomarkers including total antioxidant capacity (TAC) by FRAP method, lipid peroxidation (LPO) by Yagi , total thiol groups (TTG) by Ellman method Histological samples were also analyzed using the Nissl staining slides. Documents were analyzed by SPSS V.22 software and One Way Anova statistical test.

Results: TAC and TTG in NAC and NACNP receiving group didn't have a significant difference in comparison with control group. But about LPO, PQ poisoned group had a significant increment in comparison with NAC and NACNP treated groups ($P < 0.01$, $P < 0.05$).
Nissl staining results also declared that NAC administration whether by bulk or niosome form resulted in more alive cells in comparison with PQ group.

Discussion and Conclusion: According to the results, treatment with NACNPs leads to a partially protection against progression of PQ-challenged damages in brain in superacute toxicity.

Keywords: Acetylcysteine, Apoptosis, Brain, Nanoparticles, Paraquat

Reference:

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Screening method validation for Beta-Lactam Families of Antibiotic Residues in Milk by Biochip Array Technology and its application on real samples

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17-20 February 2021

Poster 10

Abstract Presenter:

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Introduction: Illegal and excessive use of veterinary antibiotics as a food additive for growth promoting in livestock can lead to allergic reactions and antibiotic resistance which is a worldwide concern.
Method: A biochip based semi-quantitative screening method of antimicrobial residues in milk was validated based on Commission Decision 2002/657/EC and the European guideline for the validation of screening methods for veterinary medicines. This multi-analytical screening method enables the determination of 3 β-lactams (cefalexin, ampicillin and cefuroxime) simultaneously. 47 UHT cow's milk samples collected from Tehran province, IR Iran were screened.
Results: The results showed that for all 3 antibiotic residues, the positivity threshold T was above cut-off value Fm and no false-positive results were obtained for all 3 antibiotics. All detection capabilities (CCβ) were below Maximum Residue Level (MRL) authorized by European Commission (100 µg/kg for cefalexin and 4 µg/kg for ampicillin in milk). Compliance was found in 100% of samples (47 of 47).
Discussion and Conclusion: This study found that the biochip method is valid to determine antibiotic residues in milk samples at the measured validation levels. The method was found to be fast, simple and able to screen simultaneously 3 families of β-lactams from a single milk sample with almost no sample preparation.

Keywords: β-lactams, milk, Validation, Biochip, Screening, Decision 2002/657/EC
References:1. European Commission. Commission Decision of 12 August 2002 implementing Council Directive 96/23/EC concerning the performance of analytical methods and the interpretation of results. (2002) 8–36.

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Sponge Dysidea Avara induction of ROS mediated apoptosis in human glioblastoma cells via mitochondrial targeting

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17-20 February 2021

Poster 11

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Introduction: Glioblastoma is the most lethal brain tumor with poor prognosis which possesses a high resistance against anticancer drugs. Marine organisms are an abundant source of bioactive molecules. Different studies on marinesponges indicated that sponge Dysidea avara, have cytotoxic effects on cancer cell lines; therefore, it is suggested that marine drugs can potentially be used as a beneficialmedicine in cancer therapy. Sponge Dysidea Avara's anti-cancer effects and associated mechanisms were assessed in brain tissues, focusing on parameters of inflammatory change and apoptosis.

Methods and Materials: Mitochondria were isolated from the glioblastoma cells by mechanical lysis and multiple centrifugations. The activity of mitochondrial complex II was assayed via the measurement of MTT reduction. The mitochondrial ROS measurement was performed using the fluorescent probe DCFH-DA. The Rhodamine 123 (Rh 123) redistribution technique was used for MMP measurement. Mitochondrial swelling was measured spectrophotometrically in duration 1 hour. Caspase-3 activity was evaluated using the Sigma caspase-3 assay kit. Data were analyzed using the Graph pad prism software, version 7.

Results: Our results demonstrated that Dysidea Avara induced a rise in mitochondrial reactive species (ROS) formation and mitochondrial membrane potential (MMP) collapse before mitochondrial swelling ensued in isolated brain mitochondria. In addition, collapse of MMP and mitochondrial swelling produced release of cytochrome c via outer membrane rupture or mitochondrial permeability transition (MPT) pore opening. Furthermore, caspase-3 activity was significantly increased in cells isolated from the brain when incubated with Dysidea Avara.

Discussion and Conclusion: The present study concluded that Dysidea Avara could be a potential anticancer agent. However, additional studies are needed to clarify involved mechanisms.

Keywords: glioblastoma, mitochondria, Dysidea avara, apoptosis

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Antihypertensive and Antioxidant Effects of *Sargassum angustifolium* Ethanol Extract on Cadmium Chloride-Induced Rats

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17-20 February 2021

Poster 12

Abstract Presenter:

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Introduction: *Sargassum angustifolium* is a brown alga in southwestern coastline of Persian Gulf. Regarding the presence of various bioactive compounds and evidence of antihypertensive effects in other species of *Sargassum*, we evaluated the effect of *S. angustifolium* ethanol extract in CdCl2-induced hypertension in Wistar rats.

Methods and Materials: Alga extract was prepared by maceration method using 70% ethanol and assessed for total phenolics and salt content. CdCl2 (1.5 mg/kg/day) was administered intraperitoneally to the rats for two weeks. Treatment groups *received S. angustifolium* extract (20, 40 and 80 mg/kg) or nifedipine (10 mg/kg) orally and simultaneously were given CdCl2 for two weeks. Systolic blood pressure (SBP) and heart rate were measured using tail-cuff method. Total antioxidant capacity, urea, creatinine, electrolytesincluding sodium, potassium, calcium and chloride were estimated in blood samples. The weight and histopathology of kidney tissues were also evaluated.

Results: The content of total phenolic as gallic acid equivalent and the salt as NaCl was 67.42 ± 9.5 mg/g and 6.9 g/100 g in dried ethanol extract, respectively. CdCl2 caused significant increase in SBP, kidney/body weight ratio, serum sodium and urea level and decrease in plasma total antioxidant capacity, and also histopathological alterations in kidney tissues. Treatment with *S. angustifolium* extract at the doses of 40 and 80 mg/kg significantly reversed hypertension and improved kidney weight, urea level and electrolyte changes, and enhanced antioxidant capacity and prevented histopathological changes of kidney.

Discussion and conclusion: Findings of the present study indicated antihypertensive and antioxidant effects of S. angustifolium extract against CdCl2-induced hypertension in rats.

Keywords: hypertension, cadmium chloride, antioxidants, Sargassum

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Measurement and comparison of acrylamide content of potato chips prepared by traditional and industrial methods by LC-MS/MS

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17-20 February 2021

Poster 13

Abstract Presenter:

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Introduction: Acrylamide as a possible human carcinogenic compound which is produced in carbohydrate-rich foods by high-temperature thermal processes. Potato chips (Crisps) are one of the food products that are highly prone to acrylamide formation and have a high tendency to be consumed in children and teenagers. The purpose of this study was to measure and compare the amount of acrylamide in various types of industrial and traditional potato chips produced in Tehran, Iran.

Methods and Materials: In this study, 120 samples of potato chips were randomly collected, extracted, cleaned up and their acrylamide content was measured by using a validated HPLC-Mass method. Deuterated acrylamide (d3) was used as an internal standard in the method. Result Calibration curve was linear over the concentration range of 40-400 µg/kg and the correlation coefficient was 0.999, the average recovery rate was 98.93% and the coefficient of variation was 8.95%. Limit of detection (LOD) and limit of quantification (LOQ) were 5 and 40 µg/kg, respectively. In total 120 samples were examined, and the result showed that the average amount of acrylamide in samples is 27.83 µg/kg. The average levels of contamination in the samples of industrial and traditional potato chips in 2020 were 31.85, 20, respectively, and in 2016, 31.27, 25.08 µg/kg, respectively.

Discussion & conclusion: Given the above findings, if an adult person consumes 11 g chips per day, daily average intake of acrylamide is estimated 0.00437 µg/kg body weight that is equal to 0.1% of average intake of acrylamide through all food based on JECFAs' Study in 2017. The method developed in this study is a quick, accurate and sensitive method, which also doesn't require employing special equipment in the extraction and cleaning steps. This method can be utilized to measure the amount of acrylamide in all type of potato chips.

Keywords: Potato chips (Crisps), LC-MS/MS anlysis, Acrylamide, iran, Method validation

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Evaluation of synergism effect of combinational treatment of epicathechine and edaravone in Parkinson model induced by 6-Hydroxydopamine in male rats

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17-20 February 2021

Poster 14

Abstract Presenter:

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Introduction: Parkinsons disease is a common neuropathological disorder caused by degeneration of dopaminergic neurons. The aim of this study was to investigate the evaluation of combinational treatment of epicathechine and edaravone with Madopar on behavioral effects of Parkinson model induced by 6 -Hydroxydopamine in male rats.

Methods and Materials: In this study, 40 male Wistar rats weighing 200-250 g randomly were divided into 5 groups of 8. Sham group did not receive any lesions or treatments;the Parkinsons group received unilateral injection of 4 micrograms of neurotoxin 6-hydroxy dopamine,the third group received Epicatechin (50 mg / kg, ip) and Edaravone (10 mg / kg, ip) for 14 days after brain lesions , the fourth group Madopar (50 mg / kg, gavage) and the fifth group Epicathechine -Edarvon-Madopar .after 14 days of treatments, Also a negative control considered without lesions and only received Normal saline 0.5% as vehicle .After treatments ,behavorial tests including balance test (narrow beam test), apomorphine-induced rotational test and open field test were performed.

Results: Injection of 6-hydroxy dopamine cerebroventcularly caused a significant increase in number of rotations induced by apomorphine, also total balance test times was increased and changes in open field test indexes have been occurred compared with control group.

Discussion & conclusion: According to the results of this study, combinational therapy of Epicatechin-Edaravone with Madopar improved the behavioral changes in Parkinson's model in rat

Keywords: Parkinson, Epicathechine, Edaravone

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Investigation of the therapeutic effect of nicotine and its metabolites on learning and memory

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17-20 February 2021

Poster 15

Abstract Presenter:

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Introduction: The effect of Cotinine, active metabolite of nicotine, on Aβ1-42 neurotoxicity was investigated. Cotinine possesses a longer plasma half-life, lower toxicity and it is a partial agonist of the nicotinic acetylcholine receptors (nAChR). Cotinine prolonged the survival of cortical neurons exposed to Aβ1-42. These results indicated that cotinine has a neuroprotective effect by inhibition of the formation of amyloid beta in the brain. The nicotine and its metabolites function in the brain are controversial.
In this review, the mechanism of nicotine and the metabolites on neuronal physiology were studied, also their effects on learning and memory were investigated.

Discussion & conclusion: Some studies indicate the pharmacological action of nicotine in the treatment of Parkinsons disease. There are three nicotine active metabolites that have pharmacological effects in some parts of the brain, such as cotinine, norcotinine, nornicotine, also cotinine, and nornicotine both had beneficial effects in learning and memory without adverse effects

Keywords: nicotine, Alzheimer, cotinine

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Design and synthesis of new 3-(4-methyl phenyl)-2-benzylthio-1,3-benzdiazinane-4-(3H)-one derivatives with potential anticancer effects

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17-20 February 2021

Poster 16

Abstract Presenter:

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Introduction: Cancer is a disease caused by changes in the control of the mechanisms that govern cell proliferation and cell differentiation. Cancer cell metastases and malignant tumor cells are due to abnormalities caused by hereditary factors, environmental factors such as chemicals, UV, infectious agents such as HIV. Six-membered nitrogen heterocyclic compounds received special attention in synthetic organic chemistry due to their biomedical activities. The structure of quinazoline and quinazolinone, covers a wide range of biological activities, especially in the treatment of cancer. Chemotherapy has limitations such as side effects and high cost. So there is a demand for novel drugs from alternative scaffolds. Based on this, in this research novel derivatives of 3-(4-methyl phenyl)-2-benzylthio-1,3-benzdiazinane-4-(3H)-one were designed and synthesized as anticancer agents.

Methods and Materials: Target compounds were synthesized in two steps. In the first step, 2-aminobenzoic acid and 4-methyl phenyl isothiocyanate in combination with triethylamine as a catalyst were refluxed in ethanol for 8 hours. After the completion of the reaction, the resulting product was obtained and recrystallized with ethanol. In the second step, appropriate benzyl halides were added to the solution of the resulting product in methanol and NaOH as a catalyst. After the completion of the reaction, the resulting precipitates were filtered off and recrystallized with ethanol.

Results: A series of novel 3-(4-methyl phenyl)-2-benzylthio-1,3-benzdiazinane-4-(3H)-one derivatives were synthesized in good yields and the structure of the compounds was confirmed by IR, 1H-NMR, and ESI-MS spectroscopy.

Discussion and Conclusion: In this study new derivatives of 1,3-benzdiazinane-4-(3H)-one was synthesized in two steps. Molecular structures of the synthesized compounds were confirmed by IR, 1H-NMR, and ESI-MS spectroscopy. The anticancer activity of these compounds is under investigation.

Keywords: Anti-cancer effects, Synthesis, Design, Benzdiazinane

References:

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Design and Synthesis of 3 - (4 – methoxyphenyl)- 2 – benzylthio-1, 3-benzdiazinane – 4(3H) – one derivatives with potential anti-cancer effects

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17-20 February 2021

Poster 17

Abstract Presenter:

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Introduction: Quinazolinone derivatives, an important class of heterocyclic compounds, possess a wide range of biopharmaceutical activities, including antifungal, antibacterial, anti-inflammation anti HIV, and anticancer properties. Owing to the current interest on quinazolinones as anticancer agents, our attention was attracted to synthesis of novel thioquinazolinone derivatives to develop a more potent lead molecule. Based on this, in this investigation, a new series of 3- (4- methoxyphenyl)- 2-benzylthio-1,3-benzdiazinane -4- (3H)- ones was designed and synthesized with potential anticancer effects.

Methods and Materials: A mixture of anthranilic acid, 4- methoxyphenyl isothiocyanate, and triethylamine as an efficient catalyst in ethanol was refluxed at 80 ˚C for 4-5 h. After cooling to room temperature, the resulting products were recrystallized with ethanol and used as an intermediate for synthesis of subsequent derivatives. The target thioquinazolinone derivatives were obtained via the reaction of the resulting key intermediate with appropriate alkyl halides in the presence of NaOH in methanol at room temperature. **Results:** All the target compounds were synthesized in good to high yields and the chemical structures were confirmed by IR, 1HNMR and ESI-MS spectra.

Discussion and Conclusion: A novel series of 3- (4- methoxyphenyl)- 2-benzylthio-1,3-benzdiazinane-4- (3H)- ones was designed and synthesized as anti-cancer agents in good yields. The target compounds were characterized via IR, 1HNMR and ESI-MS spectroscopies. The anticancer activity of the target compounds is under investigation.

Keywords: Design, Anticancer, Benzdiazinane, synthesis

References:

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Design and Synthesis of new 2-(alkylthio)-3-phenylquinazolin-4-one derivatives with potential anti cancer effects

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17-20 February 2021

Poster 18

Abstract Presenter:

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Introduction: Cancer is a progressive disease that involves a variety of tumors. It can also spread through tissue, lymph system, and bloodstream in the body during the metastatic process and cause tumors in other areas.There are also different drugs that can be used alone or in combination with other drugs. Due to their limited effectiveness or side effects, the use of these compounds faces problems. As a result, the synthesis of new anti-cancer compounds is of particular importance. Therefore, in this research a novel series of quinazolinone derivatives were designed and synthesized as anti-cancer compounds.

Methods and Materials: A mixture of anthranilic acid and phenyl isothiocyanate was refluxed in ethanol at 80℃ with triethylamine as a catalyst. The resulting product was recrystallized with ethanol.To a solution of the resulting product in methanol and NaOH appropriate alkyl halides were added and the solution was stirred at room temperature. After the completion of the reaction, the resulting precipitates were filtered off and recrystallized with ethanol. R: X: .Cl .Br

Results: In this study,different derivatives of quinazolinone were designed,synthesized and purified using different crystallization methods and the structure of the synthesized compounds was confirmed by IR,1HNMR and LC-MS(ESI).

Discussion and Conclusion: We designed and synthesized some novel 2-(alkylthio)-3-phenylquinazolin-4-one derivatives as anticancer agents.The structure of synthesized compounds was confirmed by IR, LC-MS(ESI), 1H-NMR, Spectroscopies .The anti-cancer activity of novel compounds is under investigation.

Keywords: Synthesis, Anti-Cancer, Quinazolinone, Design

References:

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Cyclohexylammonium salt based on 1-ethylxanthine. The first findings of preclinical studies.

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17-20 February 2021

Poster 19

Abstract Presenter:

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Introduction: To present the first stage findings in preclinical studies of the cyclohexylammonium salt of 2 - [3-methyl-7-(dioxothietanyl-3) - 1-ethyl-xanthinyl-8-thio] acetic acid.

Methods and Materials: Thromboelastography was carried out with apparatus TEG 5000 (United States). The analysis of the thromboelastograms defined general tendency of coagulation (R), functional activity of platelets and fibrinogen (MA, Angle), activity of fibrinolysis (CLT) and the physico-mechanical properties of the formed clots (G). 0.2 M CaCl2, recombinant tissue factor, and thrombin were used as TEG activators at different stages of the study. The platelet aggregation function was studied using the Born method on an AT-02 aggregometer (Russia). In the function of platelet aggregation inducers the researchers used adenosine diphosphate (ADP) at a concentration of 20 mg/ml, collagen at a concentration of 5 mg/ml, epinephrine at a concentration of 5 mg/ml, and ristomycin at a concentration of 10 mg/ml produced by Technologiya-Standart (Russia) at different stages of this study. Cytofluorimetric analysis was carried out on the BD FACSCanto II device (USA), using the "FACSDiva" software. For a marker of platelet activation, the expression of P-selectin on the platelet surface was measured by monoclonal CD62 antibodies labeled with APC (alophycocyanin) (USA)

Results: The cyclohexylammonium salt of 2 - [3-methyl-7-(dioxothietanyl-3) - 1-ethyl-xanthinyl-8-thio] acetic acid under in vitro conditions exhibits antiaggregational activity exceeding the parameters of the comparison drug.

Discussion and conclusion: The mechanism of antiaggregational activity is the inhibition of platelets release reaction. Further research is underway.

Keywords: derivatives of 1-ethylxantine, platelets release reaction, antiaggregation activity, Ant inflammation, Rat

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Application of stable isotope-labeled compound for determination of amino acids and acylcarnitines in plasma using a surrogate analyte approach and liquid chromatography-mass spectroscopy

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17-20 February 2021

Poster 20

Abstract Presenter:

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Introduction: The amount of acylcarnitines and amino acids in plasma are related to many metabolic diseases, which makes them valuable biomarkers for clinical diagnosis. As a result, many studies have been performed to determine the amounts of acylcarnitines and amino acids in plasma. Mass spectrometers are the best detector to detect and quantify these biomarkers in plasma due to the small amounts of these biomarkers. However, one of the main challenges in the analysis of plasma is the matrix effect, which can alter the result of the analysis. To overcome this problem, internal standardization methods are. On the other hand, since amino acids and acylcarnitines are endogenous molecules in biological samples, it is impossible to obtain a blank sample. The application of stable isotope-labeled compounds in a surrogate analyte approach can be a solution for all the mentioned challenges together. This study proposes a method to detect and determine the amounts of amino acids and acylcarnitines in plasma.

Methods and Materials: A surrogate analyte method by liquid chromatography-tandem mass spectroscopy (LC-MS/MS) technique was chosen using deuterium-labeled amino acids and acylcarnitines. To perform the experiment, a mixed solution of surrogate standards (SSs) in acetonitrile was prepared. Methanol/water (80/20) containing a fixed amount of SSs were added to the plasma to perform the extraction and build the calibration curve. The solutions were dried, and butanol HCl (3N) was added to the dried sample. The natural and SSs were derivatized by incubation at 65 °C. Finally, samples reconstituted by adding 1000 µl of acetonitrile/water and formic acid. The HPLC separation was performed on C8 reverse phase column and gradient of water and acetonitrile as the mobile phase. To detect the compounds, AB Sciex 4500 mass spectrometer in multiple reaction monitoring mode was used. The method was validated and MultiQuant software was used to process data.

Result: The validation results showed selectivity, linearity, accuracy, and precision. Limit of detection and limit of quantification were different for each molecule.

Discussion and conclusion: The surrogate analyte approach can be used for detection and determination of acylcarnitines and amino acids in plasma samples.

Keywords: LC-MS/MS, acylcarnitines, amino acids, surrogate analyte approach

References:

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Identification And Quantification of Three Amino Acids from Veterinary Nutritional Supplements by Using High-Performance Thin-Layer Chromatography

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17-20 February 2021

Poster 21

Abstract Presenter:

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Introduction: The present study deals with identification and quantification of three amino acids; L-lysine, L-Methionine and L-threonine using High Performance Thin Layer Chromatography (HPTLC) in two different nutritional veterinary supplements. Separation was good in the mobile phase of 1-butanol/glacial acetic acid/water (6:2:2) and densitometric determination of these compounds were carried out at 510 nm after derivatization with ninhydrine in absorbance mode.

Methods and Materials: A Camag HPTLC system equipped with an automatic TLC sampler, TLC scanner 3 (WinCATS version 1.2.3) with UV cabinet, and twin trough glass tank was used for the analysis. TLC plates of 10 cm*20cm long, precoated with silica gel 60 F254, 0.2mm thickness (Merck) were used for analysis. 100 µL syringe (Hamilton) was used for spotting the sample. The samples were applied using automated TLC sampler. CAMAG glass twin trough chamber was used for the plate development which is further scanned using CAMAG TLC scanner 3 linked to WinCAST Software (Camag, Switzerland). All chemicals used were of analytical grade. 1-Butanol, glacial acetic acid, isopropanol, and ninhydrine were obtained from Merck. Deionized distilled water was used throughout the experiment. For amino acid determination, 1g of the powdered sample was mixed with 10 ml water by sonicating for 10 min. It was then filtered and the filtrate was used for identification and quantification.

Results: The mobile phase was selected empirically using prior experience and literature reports of similar separations as a guide(1) . In order to develop an effective solvent system for the simultaneous separation of amino acids, the analysis was first tried on HPTLC plates using various combinations of mobile phase like 4:2:2, 6:3:3,6:3:1 (1-butanol/glacial acetic acid/water). It was observed that, the 6:2:2 gave the best resolution. The plate was visualized at wavelength of 510 nm. Direct quantification using a densitometer is most common method currently used by HPTLC analysis. The Rf (retardation factor) values of the amino acids and color of zones detected with ninhydrin reagent. The absolute and relative quantities of free L-amino acids were determined from veterinary nutritional supplements and the data resulting from quantitative determinations in mg amino acid /g of product (dry weight of samples).

Discussion and conclusion: The present HPTLC method is rapid, sensitive, and accurate for the simultaneous determination of five amino acids, which suggests HPTLC can be a powerful tool for the analysis of components of nutritional supplements.

Keywords: HPTLC, QUANTIFICATION, IDENTIFICATION, DENSITOMETRY, AMINO ACIDS

References:

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Design, Synthesis and Molecular Modeling of Some 1,2,4-Oxadiazole Derivatives as Novel Urea-Based Inhibitors of Soluble Epoxide Hydrolase

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17-20 February 2021

Poster 22

Abstract Presenter:

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Introduction: Human soluble epoxide hydrolase (sEH) enzyme converts Epoxyeicosatrienoic acids (EETs), substrates formed by epoxygenases from arachidonic acid, to the corresponding less active diols. Since EETs have wide range of physiological effects such as vasodilatory action and modulation of adhesion molecule expression, platelet aggregation, vascular smooth muscle migration and thrombolytic properties. Inhibition of sEH enzyme that leads to accumulation of active EETs provides a novel approach to the treatment of hypertension, atherosclerosis and inflammation. Since the most reported potent sEH inhibitors have limited pharmacokinetic profile, they are not useful for clinical application. In this study, according to the pharmacophore model suggested for sEH inhibitors, some novel compounds with 1, 2, 4 oxadiazole ring were designed. In the represented structures, the urea group is the primary pharmacophore (P1) and the 1,2,4-oxadiazole rings are considered as secondary pharmacophore (P2). P1 and P2 are linked together with a phenylene ring (L1) as a lipophilic spacer and the terminal phenyl plays the role of lipophilic pharmacophore (L2/P3).

Methods and Materials: Benzonitrile was reacted with hydroxylammonium chloride in EtOH/H2O in the presence of NaHCO3 to give corresponding amidoxime. The latter was refluxed in toluene in the presence of 4-nitrobenzoylchloride and a few drops of pyridine to yield 1,2,4-oxadiazole ring. After reduction of the nitro group in the presence of SnCl2 in ethanol and reaction with substituted phenylisocyanate new urea derivatives were achieved. Finally, the structure of compounds were confirmed using FTIR, Mass, HNMR

Results: Docking study reveals that the the designed compounds had high affinity to the active site of the sEH enzyme in comparison with 12-(3-Adamantan-1-yl-ureido)-dodecanoic acid (AUDA), a potent urea-based sEH inhibitor and has a suitable distance from the three amino acids of Tyr383, Tyr466 and Asp335 for effective hydrogen bonding.

Discussion and conclusion: In this study, according to the suggested pharmacophore model for sEH inhibitors, some novel compounds with 1,2,4 oxadiazole ring as a second pharmacophore were designed. The designed compounds showed high affinity to the active site of the sEH enzyme in the docking studies. Compounds were synthesized through 5 steps with appropriate yield and structures of these analogues confirmed by HNMR, Mass, IR.

Keywords: Oxadiazole, Soluble epoxide hydrolase, Inhibitor, docking, Synthesis

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Antidepressant-like effect of a new 3-substituted thietane 1,1-dioxide derivative in tests of neuropharmacological interaction

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17-20 February 2021

Poster 23

Abstract Presenter:

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Introduction :3-ethoxythietane-1,1-dioxide (N-199/1) is a novel molecule, which showed antidepressant activity in our previous studies (1).

Methods and Materials: We studied the mechanism of action of N-199/1, using tests with antagonists of 5HT1a- (way100635), 5HT2a/2c- (ketanserin), 5HT3- (ondansetron) and α2-receptors (yohimbine).

Results: Ketanserin potentiated the effect of N-199/1 on depression index, and yohimbine partially antagonized the effect of N-199/1 on immobility time in the forced swimming test.

Discussion and conclusion: N-199/1 causes antidepressant effect via blockade of 5HT2a/2c-receptors, and probably has slight affinity to α2-adrenoreceptors.

Keyword: thietanes, antidepressant, outbred mice, 5HT antagonists, adrenergic alpha2 antagonists

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Design and Synthesis of Novel Succinic Acid Derivatives as Fatty Acid Amide Hydrolase Inhibitors

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17-20 February 2021

Poster 24

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Introduction: Endocannabinoids, which affect CB1 and CB2 receptors, is one of the first defense lines against neuropathic pain. Fatty acid amide hydrolase (FAAH), a member of amidase enzyme, is responsible for breaking down endocannabinoids. Therefore, FAAH inhibitors may be a promising treatment for some ailments such as pain, anxiety, inflammation, and sleep disorders. (1,2). In this research, novel succinic acid derivatives as fatty acid amide hydrolase inhibitors were designed and synthesized.

Methods and Materials: Initially, 4-hydroxybenzoic acid was obtained by intense heating of the alkaline salicylic acid salt at temperatures above 240 °C for 90 min. 4-(alkoxy) benzoate was achieved by the reaction of 4-hydroxy-benzoic acid with methanol in acidic media followed by treatment with alkyl iodide in the presence of NaI and K2CO3 through nucleophilic substitution in pressure vessel at temperatures above 110 °C. The obtained esteric compound converted to corresponding hydrazide, which reacted with succinic anhydride at mild condition to produce final compounds. Interestingly, in docking study, the carboxylic acid group of the compound can form ionic interaction with Lys142 and acyl hydrazide moiety has a suitable distance from the two critical amino acids of Ser193 and Ser217 for effective hydrogen bonding.

Results: In conclusion, regarding the structure-activity relationship of fatty acid amide hydrolase inhibitors, the novel succinic acid derivatives were designed and synthesized.

Discussion and Conclusion: These compounds showed desirable affinity to the enzyme's active site in docking study and were synthesized and structurally evaluated by IR, Mass, 1HNMR, and 13CNMR spectra.

Keywords: Succinic Acid, Fatty Acid Amide Hydrolase, Synthesis

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Quantification of pregabalin by the method chromatography spectrophotometry

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17-20 February 2021

Poster 25

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Introduction: Over the past ten years, there have been cases of use of a powerful analgesic and antiepileptic drug "Pregabalin" by toxic addicts in order to obtain a narcotic effect. Pregabalin is (S) -3- (aminomethyl) -5-methylhexanoic acid. An analysis of recent studies shows that an increasing number of patients are taking doses on their own that exceed the recommended ones to achieve a euphoric state [1,2]. Pregabalin addiction is difficult to recognize in a timely manner. It is rapidly absorbed, especially on an empty stomach, does not form conjugates with plasma proteins and practically does not undergo biotransformation in the body [3].
Development of a method for the quantitative determination of pregabalin by chromatography-spectrophotometry for chemical and toxicological studies.

Methods and Materials: The objects used were a standard sample of pregabalin, a model urine mixture of a volunteer who had not taken a drug for two months, with the addition of a standard solution of pregabalin in an amount of 0.1 mg / ml.
To clean the resulting extract, a set for thin-layer chromatography "Sorbfil PTLCH-AF-A-UF" (Russia) with a size of 15x15 and "Kizilgel-60" (Germany, Merck) with a size of 20x20 was used. The quantitative determination was carried out on an spectrophotometer-2000 in the wavelength range 200-700 nm, with a cuvette layer thickness of 10x10 mm.

Results: To develop a technique for TLC-UV spectrophotometry, urine was used with an active ingredient content of 0.1 mg / ml, which was further isolated by liquid-liquid extraction.
For quantitative determination, pregabalin was preliminarily purified from concomitant endogenous substances in the urine by thin layer chromatography in a solvent system consisting of 96% ethanol-isopropyl alcohol-25% ammonium hydroxide solution (20: 10: 0.5). Next, the colored adsorption zone was eluted with acetone and its quantitative content was determined by spectrophotometry in the visible region of the spectrum at a wavelength of 567 ± 2 nm.
To establish the dependence of the optical density of pregabalin on the concentration at the selected wavelength of 567 nm, a calibration graph was built, which is linear within the concentration of pregabalin 0.01-0.06 mg / ml. According to the results of validation, it was found that the developed method is identical for the quantitative determination of pregabalin isolated from biofluid, is characterized by high reproducibility (± 2.64%), the correlation coefficient of the regression graph is r 0.9997.

Discussion and Conclusion: The best separation was obtained with the mobile phase of the composition: 96% ethyl alcohol-isopropyl alcohol-25% ammonium hydroxide solution (20: 10: 0.5). The reliability of the method was confirmed by determining the yield of the drug within 69.76% and relative standard deviation ± 2.64%.

Keywords: pregabalin, liquid-liquid extraction, thin layer chromatography, spectrophotometry in the visible region of the spectrum

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Development of A Propafenone Isolation Procedure from a Biological Fluid

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17-20 February 2021

Poster 26

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Introduction: A technique has been developed for isolating propafenone from a biological fluid for chemical and toxicological studies. As a result of the research carried out, diethyl ether was selected as an extractant. At pH = 11.77, the analyte is recovered with a yield of 65.19%, the relative mean error of the result is ± 3.04%. Propafenone is an IC class (membrane stabilizing) antiarrhythmic agent, sodium channel blocker. It is the main active ingredient of the drugs Propanorm, Ritmonorm, Ritmol. Its pharmacological effects are widely used in the treatment of various heart diseases such as supraventricular tachycardia, incl. with Wolff-Parkinson-White (WPW) syndrome; ventricular tachycardia [1- 2].
In the available literature, there is a description of cases of human poisoning with propafenone. It can cause the development of acute poisoning [3] .
The existing methods for the isolation and determination of propafenone and structurally related compounds in biological material have insufficiently high rapidity and selectivity, are distinguished by the laboriousness and complexity of the equipment used.
Purpose: Development of optimal conditions for the isolation of propafenone from biofluid.

Methods and Materials: The object of the study is the propafenone substance of the company "Xian Zelong Biotech Co., Ltd" with a basic substance content of at least 99.5% (No. 19992303115), a model mixture containing 4 mg / ml standard sample of the propafenone witness substance, Spectrophotometer-2000 ("Spectrum", Russia), pH meter ("pH-150MA", Belarus), chemical pure solvents and reagents.

Results: To develop an optimal technique for isolating propafenone from urine, we initially studied the effect of various factors on the substance yield: the nature of the solvent, the pH of the medium, the time and frequency of extraction on the isolation of propafenone from biological fluid.
Ethyl acetate, benzene, toluene, chloroform, and a mixture of butyl acetate-butanol (9: 1) were tested as the recovered liquid. To create the pH of the medium, a 0.1M solution of hydrochloric acid and a 0.1M solution of sodium hydroxide were used. The calculation of the degree of extraction (X,%) was carried out according to the specific absorption index at a wavelength of 360 nm.
It was found that the optimal organic solvent for the extraction of propafenone from solutions is diethyl ether, in which the test substance is extracted at pH = 11.77 in the maximum amount.
Discussion and Conclusion: As a result of the research carried out, diethyl ether was selected as the most optimal extractant. At pH = 11.77 with a double infusion of the biological fluid, the substance yield is 64.13–65.19%, with a relative average error of the result of ± 3.04%.

Keywords: propafenone, isolation, chemical and toxicological analysis, diethyl ether, medium pH, biolliquid.

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Evaluation of analgesic and anti-inflammatory effects of *Scutellaria nepetifolia* Benth. using pharmacological models in rats

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17-20 February 2021

Poster 27

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Introduction: *Scutellaria nepetifolia* (Boshghabi-e-Alvandi in Persian) belongs to the Lamiaceae family is an endemic species in Iran. Some other *Scutellaria* plants are very well-known for anti-inflammatory activity used in oriental medicine. They have been shown to exhibit antispasmogenic, antivasoconstrictor, antihypertensive, antiplatelet aggregation, and neuroprotective effects in different cell and animal models. The aim of this study was to investigate the analgesic and anti-inflammatory effects of this plant using pharmacological models in rats.

Methods and Materials: methanolic extract from aerial parts of Sc. *Nepetifolia* prepared by maceration using solvents (petroleum ether, dichloromethane, ethyl acetate and methanol) successively. It was examined using carrageenan-induced paw edema in rat for anti-inflammatory activity and formalin-induced paw licking tests for analgesic activity. Animals in both experiments were randomly divided into three groups: standard group (normal saline), control group (Celecoxib 40mg/kg) and treatment group (Sc. *nepetifolia* extract) in 3 doses of 30, 100 and 300mg/kg**.**

Discussion & conclusion: The results showed that Sc. *nepetifolia* methanolic extract significantly decreased the pain intensity in different doses compared to the control group. It also, at test doses of 100 and 300mg/kg P.O. clearly demonstrated anti-inflammatory effects by reducing carrageenan-induced paw edema. *Scutellaria* species are source of Phenolic compounds such as flavonoids. These findings may be explained due to high phenolic content of methanolic extract.

Keywords: anti-inflammatory, analgesic activity, Carrageenan test, Formalin test, *Scutellaria nepetifolia*

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Evaluation of the analgesic and anti-inflammatory effects of *Spirulina* Spp. Using behavioral tests in rat

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17-20 February 2021

Poster 28

Abstract Presenter:

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Introduction: Spirulina is a green-blue alga of the cyanobacterial family and contains a large number of secondary metabolites with significant biological activity. In addition, spirulina is being used as a dietary supplement in the form of tablets or powder. In some species of spirulina, analgesic and anti-inflammatory effects have been observed. In this study, the analgesic and anti-inflammatory effect of polysaccharide content extracted from the supernatant and biomass of spirulina in an animal model was investigated using formalin and carrageenan tests.

Methods and Materials: A sample of spirulina was obtained from the University of Tehran and was cultured in sterile Zarrouk medium. Cultures prepared in a sterile medium, were incubated at 27°C and 16h light exposure per day for 21-25 days. The biomass and supernatant were separated by centrifugation and then were lyophilized and dried separately. The polysaccharide content of each sample was isolated by solvent extraction. In order to evaluate their pharmacologic effects, formalin and carrageenan tests were performed on rats at the doses of 30 and 100 mg/kg of the sample extracted from the supernatant and 30 mg/kg of the sample extracted from biomass. Also, ibuprofen (50 mg/kg) was used as standard treatment and control group received saline.

Result: In formalin test, treatment of rats with supernatant extract (30 and 100 mg/kg) and biomass extract (30 mg/kg) significantly reduced pain-related behavior in rats. Moreover, treatment of rats with supernatant extract (30 and 100 mg/kg) significantly reduced carrageenan-induced paw edema compared with the control group three and four hours after carrageenan injection. Also, treatment of rats with extracted sample from the biomass (30 mg/kg) significantly diminished carrageenan-induced paw edema, both at 3h and at 4h after carrageenan injection compared with the control group

Discussion & conclusion: Our results suggest that the polysaccharide fractions extracted from the supernatant and biomass of spirulina had significant analgesic and anti-inflammatory effects. Further experiments are required to fully purified and exactly determine the structure of extracted components and also, to suggest mechanism of analgesic and anti-inflammatory activities of the compounds.

Keywords: Cyanobacteria, Spirulina sp, Analgesics, Anti inflammation, rat

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Secondary Metabolites from *Centaurea behen L.*

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17-20 February 2021

Poster 29

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Introduction: *Centaurea behen* (Gole-Gandome-Talaei in Persian) from Asteraceae family is one of the valuable sources for potent phytochemicals and growing widely and in Iran. It was traditionally used in jaundice, kidney stone and inflammation. Previous studies showed significant antioxidant and anti-inflammatory effects for various extracts of *Centaurea behen*. The present study investigated the phytoconstituents of those active extracts. For this purpose, aerial parts of *Centaurea behen* were collected, shade dried, and powdered for extraction. The powdered plant was macerated with petroleum ether, dichloromethane and ethyl acetate, respectively. The ethyl acetate extract was analyzed through various chromatographic methods like as vacuum liquid chromatography, open column chromatography and TLC to obtain pure compounds. The structures of purified compounds were elucidated on the basis of spectral data, particularly H-NMR and C-NMR experiments. As a result, a sesquiterpene and a flavonoid glycoside were isolated from ethyl acetate extract of *Centaurea behen*.

Keywords: *Centaurea behen*, flavonoid, sesquiterpene, phytochemistry

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The effect of holothurin B on endothelial cell proliferation, migration and tubulogenesis

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17-20 February 2021

Poster 30

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Introduction: Triterpene glycosides as the most bioactive components of sea cucumbers have been considered for their various pharmacological properties especially anticancer and anti-metastasis activities. Due to the limited information on the biological properties of holothurin B as a marine triterpene glycoside, the present study aimed to examine its effect on angiogenesis and compare it with curcumin using human umbilical vein endothelial cells (HUVECs). Holothurin B was isolated from Holothuria atra and identified by different NMR and Mass spectroscopy. Cell survival was estimated using MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) technique and migration of cells by Trans-well test. Angiogenesis was evaluated in vitro by tube formation test. Holothurin B reduced HUVECs survival with IC50 value of 8.16 µg/mL. At the concentrations of 5 and 7.5 µg/mL, it significantly decreased the number of migrated cells and the average length and size of tubules, and mean number of junctions and was more potent than that of curcumin. In conclusion, holothurin B could be considered as a potent antiangiogenic constituent through suppressing endothelial cell proliferation, migration and tubulogenesis in vitro suggesting its potential for further animal and clinical investigations.

Keywords: angiogenesis, cell migration, cell proliferation, holothurin B, HUVEC

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GC-MS analysis of essential oil, total phenol and flavonoid content, antibacterial, and antioxidant activities of *Chenopodium album* and *Bassia prostrata* methanol extracts

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17-20 February 2021

Poster 31

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Introduction: Traditional medicine has always guided men in dealing with diseases. *Chenopodium album* L. and *Bassia prostrata* (M. Bieb.) from the *Chenopodiaceae* family have been used in Indian traditional medicine. *C. album* is an annual plant used as hepatoprotective, diuretic, and anthelmintic agents in traditional medicine. *B. prostrata* is an annual herb and mainly used as animal fodder. Essential oils were used in ancient civilizations as main or alternative therapy. Recent studies have proven essential oils antibacterial properties and their effects on cardiovascular disease, Alzheimer, and cancers. Polyphenols, as secondary herbal metabolites, play critical roles as anti-inflammatory and antioxidant agents, so they are beneficial for human health. Up to now, because of microorganism's genetic ability to modify gene expression and other mechanisms, antibiotic resistance is growing up.

Methods and Materials: Essential oil extraction was done by the hydro-distillation method and their compounds identified with GC/MS. The methanolic extract of these herbs was used for biological assessments. Total Phenol and Total Flavonoid Contents were determined respectively by the Folin-Ciocalteu colorimetric method and Modified Woisky and Salatino $AlCl_3$ colorimetric method. Antibacterial assays were done in 3 tests by six different strains of bacteria. The pre-evaluation of the antibacterial activities of the extracts was done using the Well-Plate method in MHA. The extracts MIC values were determined by the broth microdilution method, according to CLSI. MBC was determined in MHA medium and were incubated at 37 °C for 24 h. The Antioxidant activity of extracts measured with stable DPPH radicals and compared with gallic acid and rutin to calculate IC_{50} by GraphPad Prism 8.4.2.

Discussion & conclusion: The detection of a new potent and safe treatment from the herbal origin is an excellent progress in antibacterial infection therapies. Present investigation results represent the antioxidant and antibacterial activity of *C. album* and *B. prostrata*. These antibacterial and antioxidant properties of herbs extractions confirmed their usage cause in traditional and folk medicine. According to the results, specially anti-*Pseudomonas aeurginosa* activity of *B. prostrata*, make it necessary to separate the extraction's active compounds of these two herbs and isolate them based on their biological activity.

Keywords: *Chenopodium album*, *Bassia prostrata*, Essential oil, GC-MS, Antibacterial

References:

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Compliance of Physicians to Antimicrobial Stewardship Team Consultations and its Clinical Consequences in a Teaching Hospital

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17-20 February 2021

Poster 32

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Introduction: Antimicrobial Stewardship Program (ASP) is a set of activities that leads to choosing the best antibiotic, route, dose, and duration with the lowest side effects. According to the IDSA (Infectious Diseases Society of America) Restricting antibiotic prescription is one of the recommended main approaches of ASP to rationalize antibiotic consumption. This study was performed to evaluate the adherence, limitations, and clinical consequences of ASP.

Methods and Materials: This prospective cross-sectional study was conducted from July to November 2019 in Imam Hossein Hospital, Tehran, Iran. Based on D&T committee approval, all patients receiving pre-determined antibiotics, including carbapenems, vancomycin, linezolid, teicoplanin, and colistin, should be consulted by ASP members. All consultations for patients receiving mentioned antibiotics in internal, general surgery, neurosurgery, and orthopedic wards were followed by a trained pharmacist. Patients were visited 1-3 days and 5-7 days after the consultation and the following data were recorded for each case from Electronic Medical Records (EMR) System: acceptance or rejection of consultation starting a new antibiotic, continue of treatment with the same antibiotic, clinical consequences of the patients, and duration of hospitalization. STATA.14 was used for statistical analysis.

Results: In total, 303 consultations were done by ASP members, which 260 of them were included (43 patients were discharged with personal consent). The acceptance rate for recommendations was 86.84%. According to the recommendations, the acceptance rate of the continuation of the previous antibiotic was 96.90%, changing dose 27.27%, antibiotic discontinuation 72.0%, and prescribing new antibiotic was 56.0%. The highest acceptance rate of antibiotic discontinuation was related to carbapenems 84.0%, and the lowest was related to linezolid 33.33%. Respectively, the highest and lowest acceptance rate for consultations belonged to the orthopedic 89.42% and general surgery wards 66.66%. In second and third visits, the patients clinical signs and symptoms related to the infection including leukocytosis, fever, and drop in blood pressure were followed: •Fever was detected in 4.31% of patients.

Discussion and Conclusion: The approval rate of antimicrobial stewardship team recommendations was in an acceptable range in the Imam Hossein hospital. This program didn't have a significant negative effect on patient outcomes.

Keywords: Antimicrobial Stewardship Prog, Formulary restriction, Physician acceptance

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Study on synergistic effects of *Cynara scolymus* leaf extract with conventional NAFLD treatments

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17-20 February 2021

Poster 33

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Introduction: *Cynara scolymus* as an herb widely used in traditional medicine has been shown prominent hepatoprotective effects in several studies. Accordingly, we designed a clinical trial to investigate the synergistic effects of *Cynara scolymus* leaf extract supplementation (CLES) with conventional nonalcoholic fatty liver disease (NAFLD) treatments (metformin and vitamin E). In this study, 90 subjects were randomly divided into three treated groups including metformin-vitamin E (ME), metformin- CLES (MC), and vitamin E- CLES (EC). The treatment process was followed after 12 weeks using liver ultrasound and measurement of biochemical markers such as alanine aminotransferase (ALT), aspartate aminotransferase (AST), low- density lipoprotein cholesterol, etc. This study was approved by the Ethics committee of Kermanshah University of Medical Sciences (kums.rec.1398.437) and registered in the Iranian Registry of Clinical Trials ID: IRCT40429278A1. The obtained results showed the ALT and AST significantly reduced within all groups ($p<0.05$). The ultrasonography results showed significant improvement in the fatty liver grade change of patients within all groups. Also, the grade 0 in the MC and the EC group increased. Our results showed the co-administration of CLES with metformin and vitamin E has significant effects on NAFLD. However, to approval it, clinical studies with larger scales are suggested.

Keywords: nonalcoholic fatty liver, *Cynara scolymus*, metformin, vitamin E, clinical trial

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Investigating the role of Community pharmacists in the COVID-19 crisis and highlighting their potential for emergency preparedness

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17-20 February 2021

Poster 34

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Introduction: With the rapid and widespread spread of COVID 19, governments have been forced to make the most of the full potential of the various medical professions to meet the medical needs of their countries, and are looking for more creative ways to manage human resources. It is one of the health professions that plays a key role in responding to the current epidemic. In many communities, pharmacists are the most accessible healthcare provider and the first point of contact for patients with the healthcare system. In rural and disadvantaged communities, and in areas where there is a shortage of physicians, pharmacists may be the only health care providers immediately available to patients. Pharmacists practicing in hospitals, clinics, doctors' offices, and treatment centers are trained to treat infectious diseases and can significantly expand access to care if barriers are removed [1]. During the current epidemic, it has been recognized that public pharmacies are often the first point of contact with the health care system for people with COVID-19-related health concerns or people who need reliable information and advice. This profession has a significant potential to reduce the pressure on medical staff in hospitals. Of course, pharmacists in different countries have different activities.

Methods and Materials: In this study, a review of all databases, including ISI Web of Science, Scopus, ISC, PubMed, Google Scholar related articles were examined. We also used ALPHA. [2]

Result: Pharmacists face people in the forefront during the corona pandemic. The change in the activity of pharmacies in different countries has varied. Pharmacies play an important role in reducing the workload of hospital staff by providing tools to prevent infectious disease, as well as educating people to take care of themselves, screening sick and healthy people, injecting vaccines and diagnosing minor illnesses, and providing in-person drug delivery services. Previous studies show that more than one in ten general practitioners and one in 20 emergency physicians is a minor illness that can be managed in public pharmacies. [3]

Discussion and conclusion: Despite the strong workforce of pharmacists, it is recommended that by learning interdisciplinary skills (medicine and hygiene) according to the World Health Organization, pharmacists be prepared for emergencies such as the corona pandemic so that they can reduce some of the responsibilities of physicians and nurses.Do not face a shortage of medical staff.[4]

Keywords: emergency, pharmacist's roles, COVID-19, public health, community pharmacy, interprofessional learning

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Assessment of self-medication therapy causes among university students in 2018

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Poster 35

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Introduction: Nowadays, self-medication is one of the most important health problems and has a great expenditure on health systems. Therefore, recognition of its causes is critical to reduce and control it. Our descriptive study designed for detecting and ranking main causes of self-medication between students.

Methods and Materials: 148 students of Modarres university participated in this descriptive analytical study during 2018.data were collected by a researcher made questionnaire including demographic information and influencing factors on self-medication such as health expense, time saving, para clinic assessment, personal knowledge, access to care givers in family, physician phobia, fear of parentrals . Data were analyzed by descriptive statistics and the Chi-square statistical test, using SPSS software v.18.

Results: 92% students had an experience of self-medication during last week at least. In 88% of participants, The most important causes was expense of physician visit, the second one about 76%, was poor knowledge and attitude and the third one was presence of care givers in family as 69%. The least important factor was physician phobia as 6%.

Discussion and conclusion: based on our study, one of the most effective factors on self-medication reduction is increase knowlelge and promote attitudes and performances by popular education and training on pharmacotherapy and disadvantages of medicine usage without physician order. The next factor which must be noticed by policymakers is cultural basis improvement and family background and increase accessibility to physicians for patient with every budgeting.

Keywords:physician order**,** health system, self-medication therapy, health expense

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Organic solvent-based solubilization of anti-HER2 scFv inclusion bodies

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Poster 36

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Introduction: Overexpression of recombinant proteins in prokaryotic cells including Escherichia coli, often results in the formation of intracellular insoluble and inactive particles known as inclusion bodies (IBs). Denaturing agents (e.g. urea and guanidine hydrochloride), which completely disrupt protein structure have been routinely applied to solubilize IBs and obtain bioactive proteins. However, recovery of bioactive proteins after solubilization and refolding procedures have been not guaranteed. It was shown that IB aggregates may contain native-like secondary structures of bioactive protein molecules. To recover protein from IBs, mild solubilization agents, which preserve the existing native-like secondary protein structures in the solubilized state can be used. Organic solvents such as trifluoroethanol (TFE), n-propanol and 2-butanol are examples of mild solubilizing agents. In our previous studies, anti-HER2 scFv protein which targets the therapeutic proteins, drugs, and nanoparticles toward HER2+ cancer cells was expressed in E. coli hosts. Herein, the usefulness of different organic solvents for solubilization of anti-HER2 scFv IBs was studied.

Methods and Materials: To achieve the aim of this study, expression of anti-HER2 scFv was induced by addition of 0.25 mM IPTG at 37 °C. IBs were isolated by sonication followed by centrifugation. After washing the anti-HER2 scFv IBs, they were stored at -20 °C for further analysis. Then, different organic solvents were examined for solubilization of anti-HER2 scFv IBs. Furthermore, the effect of pH buffer on solubilization of anti-HER2 scFv IBs was investigated. Accordingly, IBs was solubilized in tris buffer containing 2 M urea as well as n-propanol, 2-butanol and TFE. Then, supernatants were precipitated using trichloroacetic acid (TCA) and analyzed by SDS–PAGE. In addition, the absorbance of supernatants at 280 nm was measured.

Results: The results of this study demonstrated that among the examined solvents, TFE in combination with 2 M urea can efficiently solubilize anti-HER2 scFv IBs. Additionally, the mild solubilizing process of anti-HER2 scFv IBs was more effective at alkaline pH.

Discussion and conclusion: Totally, mild solubilization process using TFE and alkaline pH can be used for recovery of bioactive anti-HER2 scFv protein from IBs.

Keywords: HER2, Mild solubilization, TFE, alkaline pH

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Authors Index