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THE BOOK OF ABSTRACTS

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DEVELOPMENT OF THE EXTRACTION-PHOTOMETRIC METHOD FOR QUANTITATIVE DETERMINATION OF BETA-BLOCKERS

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Introduction: In recent years there is an extensive development of the methods, in which a combination of different methods of analysis of drugs is used.
Methods: The reference standard of timolol maleate (India), batch No.20121413P, propranolol hydrochloride SPU CRS M 090710, betaxolol hydrochloride - Lusochimica S.p.A.237/14, metoprolol tartrate - F.07000048 (India), carvedilol.Analytical research was performed on an Evolution 60S spectrophotometer of Thermo Fisher Scientific company, USA, a pH-150MI potentiometer using “AXIS” ANG 200 electronic laboratory balances (Poland), measuring glassware of class A.
Results: It has been proven that chloroform solutions have the absorption maxima at the wavelength observed in the absorption spectrum for bisoprolol fumarate at a wavelength of 427 nm; timolol maleate – 426 nm; propranolol hydrochloride, betaxolol hydrochloride – 425 nm; metoprolol tartrate, carvedilol – 424 nm. It has been found that ion associates are formed in the ratio of 1:9 of bisoprolol fumarate, timolol maleate, propranolol hydrochloride, betaxolol hydrochloride, carvedilol to methyl orange, the ratio of metoprolol tartrate to methyl orange is 7:9.Subordination of chloroform solutions of ionic associates of beta-blockers with methyl orange to Beer-Lambert law is observed in the concentration of the test substances of 2.0*10-4 – 2.2*10-3%. The validation characteristics of the method for quantitative determination of beta-blockers have been determined. They are robustness (analytical solutions are stable for an hour); linearity of bisoprolol fumarate (linear regression equation Y = 0.989•X + 1.1767); timolol maleate (linear regression equation Y = 1.0375•X-3.1478); propranolol hydrochloride (linear regression equation Y = 0.9738•X + 2.3452); metoprolol tartrate (linear regression equation Y = 0.974•X + 3,0797); betaxolol hydrochloride (linear regression equation Y = 1.039•X – 3.4037); carvedilol (linear regression equation Y = 1.003•X + 0.0588). These data indicate the correctness of the given method for quantitative determination.
Conclusions: The extraction spectrophotometric method developed is quite simple, sensitive and accurate.

Keywords: pharmaceutical analysis, beta-blockers, methods, quantification, control, quality, substance

DEVELOPMENT OF THE METHOD FOR PURITY DETERMINATION OF THE STANDARD SAMPLE OF NIPAZOL BY DIFFERENTIAL SCANNING CALORIMETRY

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Introduction: The aim of this research is to develop and optimize the method for purity determination of the standard sample of propyl-p-hydroxybenzene (nipazol) by differential scanning calorimetry (DSC) as part of its certification as the standard sample of the State Pharmacopoeia of Ukraine (SPhU, RS) intended for quantitative determination.
Methods: All measurements were performed on a Star SW11.00 differential scanning calorimeter of “Mettler” company. When obtaining thermograms the conditions for sample preparation and tests such as the sample weight and sample dispersion, atmospheric composition, flow rate, and pressure varied.
Results: Measurement of the heat and melting point by DSC allows determining the content of impurities in the test sample using only a few milligrams of the test substance. The mole fraction of impurities, temperature, and the molar melting heat of the substance are related by the following equation:T=To-(RTo^2/deltHf)*x2
Conclusions: As a result of the study the optimal conditions for determining the total content of impurities in the standard samples of nipazol by DSC have been developed. In order to assess correctness of the results the metrological characteristics of the research results have been calculated.

Keywords: propyl-p-hydroxybenzene, nipazol, differential scanning calorimetry, standard sample of the State Pharmacopoeia of Ukraine

THE MACROSCOPIC STUDY OF SOPHORA JAPONICA FLOWERS

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Introduction: In accordance with the requirements of the State Pharmacopoeia of Ukraine (SPhU) performance of the macroscopic analysis is an integral part when determining the parameters for standardization of medicinal plants and development of the normative documents. Standardization of the plant raw material is a guarantee of its quality and provides the efficiency and safety when using. Despite the widespread application of Sophora japonica L. (Fabaceae family) flowers by traditional medicine there are no national normative documents for this type of the raw material in Ukraine. In modern conditions the quality control of medicinal plants can be achieved due to increase of the level of standardization and conformation of the normative base with the requirements of the European Pharmacopoeia (EPh).
Methods: To conduct the research the whole and broken dried flowers of Sophora Japanese were used. As a result of the macroscopic analysis the conformity of the raw material studied to the requirements of the European Pharmacopoeia monograph “Sophora flower” has been determined, and the following diagnostic features have been proposed.
Results: The opened flower is crumpled, rolled, and has a very thin and short pedicel. The dark green or brown, campanulate calyx is about 3-4 mm long and consists of five fused sepals with longitudinal striations at the base divided at the apex into slightly bilabiate lobes. The pale yellow or light yellowish-brown, papilionaceous type corolla is often broken and is about 10-15 mm; the upper petal is the largest, subrounded, with a reflexed apex and a bright yellow unguis at its internal base. The other four petals are oblong. There are 10 free stamens surrounding a cylindrical and curved central style
Conclusions: The experimental data determining the morphological diagnostic features of Sophora Japanese flowers were used to develop the monograph “Flowers of Sophora japonica” of the SPhU.

Keywords: Sophora japonica, macroscopic study, standardization

PHARMACOGNOSTIC RESEARCH OF UKRAINIAN SAFFLOWER FLOWERS

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Introduction: Promising source of new biological active compounds is Safflower (Carthamus tinctorius L.) - from the family Asteraceae. Safflower flower and fatty oil produce wide range of pharmacological effect, such as analgesic, cholagogic, antiinflammatory, hepatoprotective. Safflower flowers contains flavonoid pigments carthamin red carthamin yellow.
Methods: The chromatographic analysis is carried out using paper and thin layer chromatography. During the development of methods of quality control of raw materials were recorded UV spectra of alcohol solutions safflower flowers on a spectrophotometer «Evolution 60S». Determination of
Results: : Results chromatographic analysis of safflower flowers showed the presence of at least 18 phenolic compounds, 4 of which referred to the hydroxycinnamic acid derivative, 4 - to substances with chalkon nature, 4 - to derivatives of flavones and flavonols.The complex
Conclusions: : Chromatography analysis showed that Ukrainian safflower flowers has rich chemical composition, which explains the wide range of pharmacological action of drugs based on safflower. The results of chromatographic analysis of flavonoids meets EP. Results of assay of so called ‘’red and yellow pigments” as well total flavonoids meets European Pharmacopoeia’s requirements.

Keywords: safflower,

DEVELOPMENT A COMPOSITION OF COLLAGEN-ALGINATE GEL FOR USE IN THE SECOND STAGE OF WOUND HEALING PROCESS.

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Introduction: For effective healing of any wounds, their treatment should be exclusively differentiated and depend on the stage of wound healing.
Methods: Because the developed preparation must be inflicted on the damaged surface, the special requirements are pulled out to basis. Base must be physically, chemically and microbiological stable, to have neutral or weak-acid pH, have potentiating properties with respect to the selected active ingredients, or be chemically inert; not contain allergens or irritants, support and help to restore the natural hydro-lipid balance of the skin. It is to such basis is gel.As the active substances were chosen collagen and sodium alginate. When choosing a gelling agent with the help of structural and mechanical research, it was justified not to use other substances as the sodium alginate is directly to them. Excipients protrude solubilizers, emulsifiers.Analysis of the gel samples by rheological indexes performance were conducted. Structural properties of the gel was studied on a rotary viscometer
Results: Rheological researches showed that all investigated standards poses thixotropic characteristics, that provides the optimal spreadability trowelling and ability of extrusion from tubas. Also stable at storage at a room and lowered temperature.
Conclusions: As a result of researches was developed the technology of collagen-alginate gel, by rheological, structural-mechanical research confirmed the composition of the gel.

Keywords: collagen-alginate, gel, rheological, research, wounds, treatment, developed.

DOXYCYCLINE HYDROCLORIDE AND CA2+, MG2+ AND AL3+ SALTS INTERACTION RESEARCH

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Introduction: Today we can trace constant increase of the presence of several chronic diseases. Therefore a requirement for combination therapy is growing. Under the circumstances of combined therapy dissemination there is an increase in cases of unreasonable receiving multiple medications and simultaneous taking medication with food that can lead to reduction treatment efficacy, reduction bioavailability or appearance of unwanted side effects. Antibiotic tetracycline hydrochloride is a classic example of interaction with metal cations. Meanwhile, it is described in literature, that doxycycline hydrochloride doesn't undergo this type of reactions. Therefore the purpose of our research was to study interaction of doxycycline hydrochloride with salts Ca2+, Mg2+ and Al3+ using absorption spectrophotometry method in the UV-region of the spectrum.
Methods: The research objects are doxycycline hydrochloride (DC), CaCl2, MgSO4 and AlCl3. Experiments carried out in the medium of purified water and 0,1M HCl. The analytical balances «Axis» ANG 200 and spectrophotometer Evolution 60s were used as a measuring devices.
Results: Analysis of the results was carried out by comparison the spectra character of solutions DC with mentioned salts and the spectra of pure substance. In the purified water and 0,1M HCl media, the intensity of absorbance is changing at the maximum of absorption for all complex compounds. The solution of DC with AlCl3 also changes the character of the spectrum, with absorption maxima shift.
Conclusions: Research the solutions of DC with metal salts by the absorption spectrophotometry in the UV region showed that this antibiotic can enter into the reaction and form a chelate complex compounds with such cations as Ca2 +, Mg2 + and Al3 + in neutral and acidic media. As a result of our research we clear up, that DC interaction with metal salts can be clinically significant and requires further study of a bioavailability.

Keywords: doxycycline hydrochloride, metal salts, interaction, complexes.

MICROSCOPIC STUDY LEAF OF YELLOW AZALEA (RHODODENDRON LUTEUM SWEET.)

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Introduction: Genus of Rhododendron is one of the largest genera of Ericaceae family, which includes over 600 species. In Ukraine, Rhododendron luteum grows in natural conditions.
Methods: Leaves of Rhododendron luteum were collected in the Botanical Garden of Kharkov State University, fixed with 96% ethyl alcohol - glycerol - water (1:1:1). Temporary preparations ware prepared according to the standard method. The preparations were investigated using a microscope, IBI-10, at 80, 120, 300, 600 and 800-fold magnification; the photomicrographs were made by digital camera OLYMPUS FE-140.
Results: The leaf blade is dorsoventral, gipostomatic, pubescent on the edge and on both sides with simple and glandular trichomes. The upper epidermis (fig. 2) has no stomas, has basic cells with slightly winding thin sidewalls and outer layer of the cuticle. Trichomes are represented by large clavate-capitate of emergence from multicellular pedestal, multi-cellular and multi-pedicle, extending to bottom, and a multicellular secreting head. Among simple coating trichomes, 1-2-cellular ones prevail; they are sharp, thin and long, slightly twisting live hairs with 8-10-cellular rosette at the base. In addition, simple bundle emergence are found in the upper epidermis and on the edge of the leaf blade they are more densely arranged.The petiole in cross section is rounded-triangular, it comprises a large central cariniform bundle and one small lateral bundle. The large bundle has sclerenchymatous lining. Epidermis of petiole has stomata and trichomes similar to those of the leaf blade.Parenchyma is not uniform: there are many cells with large druses, as well as numerous secretory cells with orange content; there are cavities that enlarge with leaf aging.
Conclusions: Microscopic studies of Rhododendron luteum leaves make it possible to identify a set of core diagnostic features of this species, which can be used in diagnostics of medicinal plants.

Keywords: genus, leaf, trichomes (or hairs), stomatal apparatus, epidermis, glandular hair.

THE CHOICE OF EXCIPIENTS IN THE COMPOSITION OF A MEDICATED CHEWING GUM.

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Introduction: Medicated chewing gum (MCG) is a rational dosage form for the treatment of dental diseases. MCG, except active pharmaceuticals ingredients (APIs), contains chewing basis and excipients, choice of which was the aim of our work.
Methods: As object of study was chosen MCG with lysozyme hydrochloride and papain and as a gum base –HiG-01 (Cafosa, Spain). We used the following groups of adjuvants: sweetening agents, flavoring agents, glidants, lubricants, humidifiers, binders. During the development of the composition we researched physicochemical (crystal size and shape, moisture content) and technological parameters (bulk density, flowability).
Results: The results of physico-chemical and technological research of APIs and there mixture with the gum base have established the need of granulation for tabletting mass. For this purpose as humidifiers we used a solution of PVP 5% and ethanol 20%. In appearance of the obtained granules and optimal technological properties as binder component was selected ethanol 20%. To enter the liquid flavoring oil Melon in the MCG composition necessary to use moisture-absorbing agents that make it easy to transform liquid APIs in powder with good fluidity. For this purpose were used Aeros 380, Syloid® 244FP, Neusilin®, which also play a role of glidant in the manufacture of solid dosage forms. According to the results of the moisture-absorbing capacity of adsorbents and fluidity research was obtained that the best results had a mixture with Syloid® 244FP at a concentration of 1.5%. To determine the optimal flavoring agent were used xylitol and sorbitol. According to the results we selected xylitol in an amount of 0.3%, which also has anticaries effect. As anti-friction substance was selected magnesium stearate in an amount of 1%.
Conclusions: All things consider, on the basis of physicochemical and pharmacological and technological research was developed optimal composition of medicated chewing gum for use in the dental practice.

Keywords: Dental diseases, medicated chewing gum, excipitients, physico-chemical and technological researches.

COPPER COMPLEXES OF 2-HYDROXY-1,4-NAPHTOQUINONE FROM LAWSONIA INERMIS L. (HENNA) AS POTENTIAL ANTI-CANCER AGENTS

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Introduction: Lawsonia inermis L. (henna) is a pharmacologically important plant with significant biological activities including antioxidant, anti-inflammatory, antibacterial and anticancer activities. The active coloring and biologically active principle of henna is found to be lawsone (2- hydroxy-1,4-naphthoquinone). The aim of this study was to evaluate cytotoxicity of selected copper(II) complexes of lawsone and to determine their effects on the process of apoptosis on human monocyte cell line THP-1.
Methods: All the tested compounds were synthesized at the Department of Chemical Drugs, Faculty of Pharmacy, UVPS Brno. Cells were maintained in RPMI 1640 medium and treated with tested compounds at various concentrations for 24 hours. The cytotoxicity of tested complexes was evaluated by enzyme-based WST-1 method and the western blotting and immunodetection was used to detect specific proteins.
Results: Based on the IC(50) values, complexes LAW2,4, 6 and 7 showed greater toxicity than other tested compounds. Endogenous levels of anti-apoptotic MCL-1 were lower in treated cells compared to untreated control group, with the most significant decrease in cells treated with lawsone and complex LAW2. Caspase 3 (Cas-3), one of the executioner caspases was detected as 32 kDa pro Cas-3, as well as p17 subunit of the cleaved (active) Cas-3. Significant increase in p17 form was observed in samples treated with LAW4, 6 and 7.
Conclusions: All the complexes demonstrated significant cytotoxicity, which was higher compared to cytotoxicity of pure lawsone. Our data indicate that lawson-copper(II) complexes may induce the intrinsic apoptosis pathway, given that the activation of caspase 3 and modulation of apoptosis-related proteins such as MCL-1 were observed. In conclusion, lawsone-copper(II) ternary complexes may be considered to have the potential to become new antitumor agents. Although further studies are required to precisely define the mechanisms of action in human cancer cells, here their cytotoxic and pro-apoptotic effects have been demonstrated.

Keywords: lawsone, copper, apoptosis, Lawsonia inermis, caspase

PHARMACEUTICAL DEVELOPMENT OF OINTMENT FOR THE FIRST PHASE OF WOUND HEALING WITH CHAMOMILE EXTRACT CONTENT

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Introduction: Dynamic development of surgery, antimicrobial, reparative and anti-inflammatory therapies constantly put new requirements to treatment algorithms of wounds and wound infection. Wound process phasicity determines requirements for medicinal products - so, for topical treatment of phase I of wound process drugs should have a combined effect. Biologically active substances contained in thick oil extract of chamomile flowers provide anti-inflammatory, local anesthetic, antimicrobial and restorative action that creates prospects for development of ointment with its content.
Methods: The objects of the study were chamomile thick oily extract and polyethylene oxide basis. In pharmaceutical development of ointment composition used physicochemical (solubility, homogeneity), structural and mechanical (structural viscosity), biopharmaceutical (osmotic activity, the release of the BAS in agar gel), microscopy (homogeneity) and microbiological (wells method) analysis methods.
Results: Has been studied solubility of thick oil extract and grounded the use of mixed solvent for rational introduction into ointment base. When designing the composition of the ointment base by means of structural and mechanical and biopharmaceutical research methods were investigated the ointment base properties changes of on the ratio of polyethylene oxides 1500:400. All samples have a plastic flow type with high flow limit. Osmotic (absorptive) properties of model bases are 300-400% at 6th hour of the experiment. Using microscopy, the ointment homogeneity was confirmed. Has been justified the composition of ointment codenamed
Conclusions: Has been carried out pharmaceutical development of ointment for the phase I of wound process treatment. After preclinical studies the drug can be offered for practical medicine.

Keywords: Wound process, ointment, polyethylene oxide, chamomile thick oil extract.

PHARMACO-TECHNOLOGICAL PROPERTIES OF TABLET MASS AND DETERMINATION OF TABLETS WITH CONTENT OF COMPLEX DENSE EXTRACT QUALITY

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Introduction: Cardiovascular diseases rank first among the most common and dangerous diseases of our time. Cardiovascular diseases manifest differently and have various origins. Urbanization, industrialization and globalization inherent in the transition economies, promote lifestyle changes that lead to the development of heart diseases. Providing cardiovascular patients highly effective and affordable drugs is a priority for the pharmaceutical industry.
Methods: As a research object we have selected complex thick extract obtained by joint extraction of hawthorn fruit, Leonurus herb, melissa herb and hop cones. During the study used complex of pharmaco-technological research methods to determine the fractional composition, moisture absorption, flowability, bulk density, compressibility, etc. In the following the quality indicators of obtained tablets have been defined: the average weight, the mechanical strength (friability and resistance to crushing), disintegration, etc.
Results: When creating tablets model tablet formulations have been developed which included lactose, croscarmellose sodium, microcrystalline cellulose, talc and magnesium stearate. Complex thick extract was introduced in the tablet mass together with moisturizer solution which varied in its qualitative composition (Plasdone K25 solutions). As a result of studying pharmaco-technological properties of tablet masses it has been found that fractional composition of model samples makes a fraction of 1 mm 78-85% ,Hausner ratio is 24-30, Carr coefficient is 1.3-1.4, flowability 2.8 -3.4 g/s, the angle of repose is 26-33°. Based on the study of tablet masses water absorption dynamics for one day it has been determined that humidity after 24 hours makes 5.0-6.5%. The tablets obtained based on the tabletting masses studied, were subjected to the study of mechanical strength and disintegration.
Conclusions: Studies have shown that the optimal quality indicators has the tablet mass and tablets with content as a moisturizer of Plasdone K25 alcohol solution.

Keywords: Cardiovascular diseases, tablets, complex dense extract, pharmaco-technological properties, quality indicators.

DEVELOPMENT OF CAMEL'S THORN THICK EXTRACT OBTAINING TECHNOLOGY AND ITS STUDY

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Introduction: Search and creation of medicinal substances with high pharmacological activity is a primary task of pharmaceutical branch. In this regard of great interest are vegetable raw materials, which are a valuable source of biologically active substances, possessing comprehensive therapeutic action on the body. Alhagi herb is known for its healing properties since ancient times and is used in Kazakhstan folk medicine in various diseases, therefore a prospective direction should be obtaining and study of alhagi thick extract with high active components content with the purpose of medicines creation.
Methods: The object of our studies was the alhagi herb. Performing the work we used a complex of phyto-chemical, technological and microbiological analysis methods by which means was grounded the choice of extractant, studied extraction process dynamics, developed the technology of thick extract obtaining and carried out its chemical and microbiological analysis.
Results: It was found, that of used extractants (purified water, ethanol) the maximum extractive ability has 70% water-ethanol solution (19,37±0,2)%. The thick extract was obtained by filtration extraction method in laboratory conditions. As a result of extraction process dynamics study were justified extraction parameters: ratio raw:extractant 1:6, providing the yield of extractives (14,0±0,3)%, extraction rate – 3-4ml/sec. Thick extract was obtained by condensation of liquid extract on a rotor vacuum evaporator to moisture content 25%. Studying chemical composition it has been found that the thick extract contains (2,4±0,2)% flavonoid structure substances in terms of rutin. Microbiological studies have determined relatively high antimicrobial properties of the thick extract.
Conclusions: As a result of conducted research was developed the technology for thick extract obtaining, carried out the analysis of its chemical composition and described microbiological properties. The studies allow using the thick extract for creating ready medicines of antimicrobial action.

Keywords: Alhagi, extractant, extraction, thick extract, flavonoids, antimicrobial activity.

CLOPIDOGREL CONCENTRATION IN PATIENTS WITH ACUTE MYOCARDIAL INFARCTION AND IMPAIRED CARDIAC FUNCTION

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Introduction: Clopidogrel is an oral antiplatelet drug of thienopyridine class. An active metabolite of clopidogrel irreversibly inhibits platelet activation and aggregation by blocking the ADP receptor. Clopidogrel, on a background of standard care (including acetylsalicylic acid and fibrinolytic therapy) would prevent re-occlusion, enhance infarct-related artery patency, and improve clinical outcomes in patients with acute coronary syndrome.
Methods: This investigation included a total of 25 patients with acute myocardial infarction, 15 male (60.0%) and 10 female (40.0%), which were treated at Clinic of Cardiology, Clinical center in Nis. All patients were on dual antiplatelet therapy with acetylsalicylic acid and clopidogrel. Concentration of clopidogrel was measured using UHPLC-DAD-MS analysis.
Results: Clopidogrel concentration ranged from 0.30ng/ml to 83.00ng/ml, with an average of 23.28±18.58ng/ml. Using Pearson's correlation test a statistically significant strong positive correlation was registered between the plasma concentration of clopidogrel in patients with acute myocardial infarction and left ventricular ejection fraction ($r=0.540$, $p<0.005$).
Conclusions: Acute myocardial infarction is often accompanied by reduced left ventricular ejection fraction due to damage of the heart muscle. Our study has shown that in patients with impaired cardiac function after myocardial infarction, there is reduction in the plasma concentration of clopidogrel achieved.

Keywords: clopidogrel, acute myocardial infarction, ejection fraction

THE INFLUENCE OF GENETICS ON THE REVERSAL OF ANTICOAGULATION IN PATIENTS STOPPING WARFARIN PRIOR TO SURGERY.

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Introduction: Warfarin is the most commonly used oral anticoagulant for the prevention and treatment of thromboembolic disorders. According to the current guidelines, patients receiving warfarin who are scheduled for an invasive procedure are required to stop taking the drug for 5 days so that normal coagulation is resumed. However, the rate by which anticoagulation (measured by INR) subsides varies among different patients; for some INR falls either too slowly (at increased risk of peri-operative bleeding) or too fast (at increased risk of thromboembolism).The aims of this project were (i) To investigate the influence of CYP2C9 and VKORC1 polymorphisms on the rate of INR decline and (ii) to determine the relationship between the fall in INR and falling plasma concentrations of S-warfarin.
Methods: Patients completing a short course of warfarin were recruited into the study. Blood samples were collected on alternate days over 9 days for INR and plasma warfarin concentration determinations and for CYP2C9 and VKORC1 genotyping. Plasma concentration of the two enantiomeric forms of warfarin were determined using reverse-phase High Performance Liquid Chromatography (HPLC).
Results: Stepwise regression analysis revealed a statistically significant association ($p=0.02$) between the time to reach INR<=1.5 and CYP2C9 genotype. Age had a marginal effect ($p=0.06$). INR decay was significantly associated with the decline in S-warfarin plasma concentrations.
Conclusions: The fall in INR following warfarin cessation is significantly associated with CYP2C9 genotype, with the latter influencing the rate of fall in S-warfarin plasma concentrations. A pharmacogenetic-guided algorithm based on CYP2C9 genotype has the potential to accurately predict the period of time needed to stop taking warfarin in individual patients scheduled for invasive procedures.Future work includes the validation of the generated algorithm in a different cohort of patients who omitted warfarin for the purpose of a surgery.

Keywords: warfarin, anticoagulation, reversal, INR, pharmacogenetics, HPLC

APPLICATION OF FTIR-ATR SPECTROSCOPY, HPLC AND CHEMOMETRIC METHODS TO QUANTITATIVE ANALYSIS OF METHYLXANTHINES, POLYPHENOLS AND ANTIOXIDANT ACTIVITY OF YERBA MATE

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Introduction: The interest in nutraceuticals and functional food, which are demonstrated to have health benefits and reduce the risk of chronic disease, continous to grow in the recent years. The subject of our research was yerba mate. Yerba mate presents hypocholesterolemic, vasodilatory, anti-inflammatory, anti-obesity, and choleretic effects, and it is able to reduce the progression of atherosclerosis. These extraordinary health benefits yerba mate have been attributed to the its bioactive ingredients like polyphenols and purine alkaloids, mainly caffeine. The aim of study was (i) to determine of caffeine, chlorogenic acids and rutin content in yerba mate and selected dietary suplements (containing yerba mate and green coffee extracts), (ii) to determine antioxidant activity of samples, (iii) an application of multivariate calibration and FTIR spectroscopy for the quantification of active substances and antioxidant activity.
Methods: The study material comprised 20 samples of yerba mate (Ilex paraguariensis) and dietary supplements containing extracts from yerba mate and green coffee. The antioxidant activity of yerba mate extracts was determined by spectrophotometric method using the 2,2-diphenyl-1-picrylhydrazyl hydrate radical (DPPH). The content of caffeine, chlorogenic acids and rutin was determined by RP-HPLC method and DAD detector with nonpolar (C18) column in gradient mode (ACN, water + formic acid). The mid-infrared (MIR) spectra using an attenuated total reflectance (ATR) technique were recorded for dry ground samples within 400-4000 cm-1.
Results: HPLC method allowed for the identification and quantification of caffeine, chlorogenic acids and rutin in the water extracts of yerba mate and dietary supplements.
Conclusions: The multivariate calibration with PLS regression method succesfully provides the model for prediction of these compounds content as well as antioxidant activity of yerba mate samples based on FTIR-ATR spectra. The results are consistent with those obtained by the HPLC method.

Keywords: Yerba mate, Ilex paraguariensis, antioxidant activity, HPLC

TABLE OF CONTENTS