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Crne Gore**
Pharmaceutical Chamber of Montenegro



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FARMACEUTSKI FAKULTET



CALIMS

U SARADNJI SA AGENCIJOM ZA LJEKOVE I MEDICINSKA SREDSTVA CRNE GORE

**II KONGRES FARMACEUTA CRNE GORE SA MEĐUNARODNIM UČEŠĆEM
II CONGRESS OF PHARMACISTS OF MONTENEGRO WITH THE INTERNATIONAL PARTICIPATION**

ZBORNİK SAŽETAKA ABSTRACT BOOK

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PHARMACY - SCIENCE AND PRACTICE GUIDED BY HUMANITY**

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**II Kongres farmaceuta Crne Gore sa međunarodnim učešćem
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THE ROLE OF EDUCATION IN DEVELOPING HEALTH LITERACY OF YOUNG PEOPLE ABOUT EMERGENCY CONTRACEPTION

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Under the reproductive health WHO implies a state of physical, mental and social well-being of all age groups in relation to reproductive system. By this is meant a satisfying and safe sex life, ability to reproduce and opportunity to decide about reproduction. In realizing these rights, there is a big role of education of young people in gaining the knowledge and necessary informations about the maintenance of reproductive health.

The aim is to highlight the importance of education for young people within the subjects about preserving reproductive health. Young people through teaching gain attitudes and knowledge about contraception, as well as awareness about active participation in decisions related to their reproductive health. Based on this methods the possibilities are analyzed for further development and improvement of health literacy of young people about reproductive health.

During school year 2013/2014, 120 students of Pharmacy and Physiotherapy School were questioned. Students of different majors who have passed the subject of Hygiene were tested, as well as those who have remained to study that subject.

By statistical analysis of results was produced the data that students of the 1st grade within the subject Hygiene receive basic knowledge of the reproductive system and forms of contraception, while the 4th grade students who listened to the subject of Pharmacology better in answers about the activity and effects of emergency contraception on the organism.

In preservation of the reproductive health of young people is necessary to significantly improve and expand the curriculum subjects of hygiene, where the students in addition to basic knowledge about forms of contraception have gained a wider picture of usage, efficacy and side effects of emergency contraception. In schools that do not have subjects that deal with reproductive health it is necessary to introduce sexual education.

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PRIMENA RAZLIČITIH IN VITRO TEHNIKA ZA PREDVIĐANJE PERMEABILNOSTI KROZ KRVNO-MOŽDANU BARIJERU LIGANADA IMIDAZOLINSKIH RECEPTORA

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Ligandi imidazolinskih receptora predstavljaju brojnu familiju biološki aktivnih jedinjenja koja imaju široku terapijsku primenu. Ovi ligandi mogu delovati na tri tipa imidazolinskih receptora (I1-IR, I2-IR and I3-IR) i na alfa2-adreno receptore. Imidazolinski receptori su odgovorni za različite biološke aktivnosti imidazolina. Stoga neki IRs ligandi su danas značajni za ispitivanje kao novi centralno delujući antihipertenzivi i potencijalni kandidati za lečenje različitih neuroloških oboljenja. Cilj ovog rada je bio da se proceni permeabilnost ovih liganada kroz Krvno-Moždanu Barijeru (KMB).

Test permeabilnosti na veštačkim paralelnim membranama (eng. Parallel Artificial Membrane Permeability Assay, PAMPA), bioparticiona micelarna hromatografija (eng. Biopartitioning Micellar Chromatography, BMC) i reverzno-fazna tečna hromatografija pod visokim pritiskom (eng. Reversed-Phase High-Performance Liquid Chromatography, RP-HPLC) su in vitro tehnike korišćenje za predviđnje permeabilnosti kroz KMB imidazolinskih liganada. Vrednosti dobijene korišćenjem PAMPA i BMC su ispitivane metodologijom kvantitativnog odnosa struktura i osobina jedinjenja (eng. Quantitative Structure-Property Relationship, QSPR).

Retencioni faktori dobijeni korišćenjem BMC i RP-HPLC su korelisani sa koeficijentima permeabilnosti dobijeni korišćenjem PAMPA. Pored toga, PLS (eng. Partial Least Square), MLR (eng. Multiple Linear Regression) i ANN (eng. Artificial Neural Networks) modeli su razvijeni korišćenjem retencionih podataka iz BMC sistema/efektivnih permeabilnosti iz PAMPA i molekularnih parametara izračunatih za optimizovane strukture. Dominantni molekularni/katjonski oblici jedinjenja na pH=7.4 su dobijeni korišćenjem MarvinSketch. Geometrijska optimizacija liganada je izvršena korišćenjem Chem3DBio Ultra. Molekularni deskriptori za optimizovana jedinjenja su izračunati korišćenjem Chem3DBio Ultra, Dragon and ADMET predictor programa. U ovoj QSPR studiji retencioni faktori/efektivne permeabilnosti jedinjenja su korišćene kao zavisne, dok izračunati deskriptori su korišćeni kao nezavisne varijable. SIMCA je korišćena za PLS analizu dok je postupno MLR i ANN modeliranje izvršeno korišćenjem STASTICA Neural Networks programa. Prognostički potencijal formiranih QSPR modela je potvrđen ukrštenom i eksternom validacijom.

Formirani QSPR modeli mogu biti korišćeni kao brzi skrining metod za procenu krvno-moždane permeabilnosti novih liganada imidazolinskih receptora, koji predstavljaju potencijalne kandidate u lečenju hipertenzije i neuroloških oboljenja.

Ključne reči: Imidazolini, PAMPA, BMC, RP-HPLC, QSPR

APPLICATION OF DIFFERENT IN VITRO TECHNIQUES FOR PREDICTING BLOOD BRAIN BARRIER PENETRATION IMIDAZOLINE RECEPTOR LIGANDS

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Imidazoline receptor ligands are a numerous family of biologically active compounds with many therapeutic applications. Those ligands can act at the three types of imidazoline receptors (I1-IR, I2-IR and I3-IR) and alpha2-adrenoceptors. Imidazoline receptors (IRs) are responsible for the versatile biological activities of imidazolines. Therefore some IRs ligands are examined as novel centrally

acting antihypertensives and drug candidates for treatment of various neurological diseases. The aim of this work was to evaluate Blood-Brain Barrier (BBB) permeability of these ligand.

Parallel Artificial Membrane Permeability Assay (PAMPA), Biopartitioning Micellar Chromatography (BMC) and Reversed-Phase High-Performance Liquid Chromatography (RP HPLC) are in vitro techniques used for predicting BBB penetration of imidazoline ligands. The values obtained using PAMPA and BMC were studied by the Quantitative Structure-Property Relationship (QSPR) methodology.

Retention factors obtained using BMC and RP-HPLC were correlated with permeability coefficients obtained using PAMPA. Further, Partial Least Square (PLS), Multiple Linear Regression (MLR) and Artificial Neural Networks (ANN) models were developed using retention data from BMC system/effective permeabilities from PAMPA and molecular parameters calculated for the optimized compounds. The dominant molecules/cation species of compounds at pH=7.4 have been obtained using the MarvinSketch. Chem3DBio Ultra program was applied for geometry optimization. The molecular descriptors were calculated for the optimized compounds using ChemBio3D Ultra, Dragon and ADMET predictor software. Retention factors/effective permeabilities of compounds were used as dependant variable, while calculated molecular parameters were used as independent variables in the QSPR study. SIMCA was used for PLS analysis, while the stepwise MLR and ANN modeling were performed using STASTICA Neural Networks. Predictive potential of the formed models was confirmed by Leave-One-Out Cross- and external validation.

Formed QSPR models can be used as a fast screening method for assessment of brain penetration of novel imidazoline receptor ligands, as promising drug candidates for treatment of hypertension or neurological diseases.

Key words: Imidazolines, PAMPA, BMC, RP-HPLC, QSPR

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POREDENJE PUNOG FAKTORSKOG DIZAJNA, CENTRALNOG KOMPOZICIONOG DIZAJNA I BOX-BEHENKEN DIZAJNA U RAZVOJU HROMATOGRAFSKE METODE ZA ANALIZU FLUKONAZOLA I NJEGOVIH NEČISTOĆA

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Primjena savremenih hemometrijskih tehnika u razvoju metoda tačne hromatografije omogućava detaljnu analizu ispitivanog sistema i rješavanje složenih analitičkih problema koji se ne mogu riješiti jednostavnim procedurama. Metodologija eksperimentalnog dizajna (DoE) omogućava primjenu matematičkih modela s kojima je moguće predvidjeti ponašanje sistema izvođenjem minimalnog broja dobro isplaniranih eksperimenata.

Cilj ovog istraživanja je bio istovremeno poređenje četiri vrste eksperimentalnog dizajna: pun faktorski dizajn na dva nivoa (FFD 23), centralni kompozicioni dizajn (CCD), Box-Behnken dizajn (BBD) i pun faktorski dizajn na tri nivoa (FFD 33). Sve vrste dizajna primijenjene su za dizajniranje