

CONTENTS VOL. XLIV/1/2014:

AGRICULTURE AND FORESTRY SCIENCES, ANIMAL SCIENCE

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|--|-----|
| AMZOIU EMILIA, AVERIS LARISA ELISABETH, BEJENARU CORNELIA, MANUEL OVIDIU AMZOIU, PAUL GABRIEL ANOICA - The correlation studies of antimycobacterial activity for a number of derivatives of 4-carboxamide | 7 |
| AMZOIU EMILIA, BELU IONELA, AVERIS LARISA ELISABETH, AMZOIU DENISA, LUDOVIC BEJENARU - The study of partition coefficient octanol/water for 3-(2-allylsulfanyl-6-benzothiazolylaminomethyl)-2-benzoxazolione as photosynthesis inhibitors | 15 |
| BERCEA IULIAN, NICULESCU MARIANA - The influence of the density of the natural regeneration of the seedlings of hungarian (Quercusfrainetto) and turkey oak (Quercuscerris) on the individual changes of trees following the woodland stage | 21 |
| BONCIU ELENA, IANCU PAULA - Study regarding influence of the organic fertilization on the morphological and productivity traits of the soybean (Glycine max) | 29 |
| BUSE DRAGOMIR LUMINITA, NICOLAE ION - Ecophysiological aspects regarding the „Sibleac,, associations from Iron Gates Natural Park | 34 |
| BUSE DRAGOMIR LUMINITA, NICOLAE ION - Research regarding the physiology of Cotinus coggigria Scop.species | 40 |
| BUZATU CLAUDIU, GRECU FLORINA - Experimental studies on the fertility of the eutricpsamosoil in Poiana Mare – Dolj | 45 |
| CIULCA S., RENATA ȘUMĂLAN, SORINA POPESCU , BRIGITTA SCHMIDT, ȘUMĂLAN R. - Univariate and multivariate analysis of some garlic landraces for bulbs traits | 50 |
| COJOACĂ FLORIN DORIAN, FLORIN ACHIM, MARIAN STAN, SILVIU PĂUNESCU - Application of GPS tehnology (global positioning system) in forest inventory statistics | 57 |
| COLĂ MUGUREL, COLĂ FLORICA - Influence of feeding on the weight of broiler chickens | 64 |
| COLĂ MUGUREL, COLĂ FLORICA - Effect of feeding on the consumption of fodder and the structure of broilers carcasses | 68 |
| CROITORU IRINA MARINELA, CROITORU ALIN, MILUȚ MARIUS - Research on the influence of chemical fertilizers on temporary short-exploitation grassland | 73 |
| CROITORU IRINA MARINELA, CROITORU ALIN - The influence of the proportion between the components in two simple short-exploitation mixtures | 79 |
| DIMA MILICA - The influence of the climatic conditions on production of foreign varieties of peanuts grown on sandy soils | 83 |
| DURĂU CARMEN CLAUDIA, OTILIA COTUNA, VERONICA SĂRĂTEANU - Approaches on the dynamics of the floristic composition of a Banat hill grassland (Western Romania) | 87 |
| FĂGĂRAȘ MARIUS - Psammophilous plant associations from the coastal area of the Black Sea between Periboina and Periteașca (Danube Delta Biosphere Reserve) | 90 |
| GAMENT EUGENIA, MARINESCU MARIANA, ANGER ILDIKO, MIHALACHE M., ILIEL., STOICIU FL. - Effect of steel slag LF application on soil chemical properties | 102 |
| IANCU PAULA, SOARE, M., MATEI GHE. - The influence of chemical fertilisers and soil upon the crop formation to groundnuts and the correlation with the phenomenon of withering | 108 |
| ILIE L., MIHALACHE M., GINA SCĂEȚEANU - Bulk density of some romanian soils | 114 |
| IONESCU NICOLAIE, IONESCU SORIN GABRIEL - Relationships between sludge doses and calcium content from agricultural crops | 122 |
| IVAN GHEORGHE, TUDORA CATALINA - Evaluation of safflower culture (Carthamus tinctorius) as a forage alternative for sunflower culture (Helianthus annuus) in the arid areas of southern Romania | 128 |
| MARINESCU MARIANA, LACATUSU ANCA, GAMENT EUGENIA, MARINESCUM. - The influence of different treatments of soil polluted with crude oil on plant biomass | 134 |
| MATEI GHEORGHE, TORCEA MARIAN, IMBREA FLORIN - Quality assessment of tobacco type Virginia F.I. using international rating system | 140 |
| MATEI GHEORGHE, ROTARU ADRIAN, IMBREA FLORIN, ROTARU ELENA - Study on main indicators of panification of an assortment of common wheat received and stored at Boromir – Deva | 148 |
| MIHALACHE M., ILIE L., MARIN D.I., ILDIKO ANGER - Research regarding the influence of LF slag on chromic luvisol reaction and wheat yield in the experimental field from Moara Domneasca | 156 |
| MITITELU MAGDALENA, IONIȚĂ CORINA, IONIȚĂ ELENA, NEACȘU SORINEL MARIUS, AMZOIU EMILIA, AVERIS LARISA MARINA ELISABETH, MOROȘAN ELENA - Detection of heavy metals from molluscs shells | 164 |
| MITITELU MAGDALENA, IONIȚĂ CORINA, IONIȚĂ ELENA, NEACȘU SORINEL MARIUS, AMZOIU EMILIA, AVERIS LARISA MARINA ELISABETH, MOROȘAN ELENA - Investigation of heavy metals from some alimentary products | 168 |
| NICULESCU MARIANA, BERCEA IULIAN, NICULESCU LAURENȚIU, HÎRJEU NICOLETA - The forest habitats found in Lespezi Quarry, Dâmbovița County | 171 |

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|---|-----|
| NICULESCU MARIANA, BERCEA IULIAN, NICULESCU LAURENȚIU, NUȚĂ ILIE SILVESTRU - Considerations about the woody vegetation of the Băița-Crăciunești area, Hunedoara County | 177 |
| PARASCHIVU MIRELA, OTILIA COTUNA, MARIUS PARASCHIVU - Integrated disease management of Fusarium head blight, a sustainable option for wheat growers worldwide | 185 |
| PARASCHIVU MIRELA, CRISTINA BĂBEANU, RODICA SOARE, MARIA DINU, MĂDĂLINA DRĂGOI - Influence of late blight (Phytophthora infestans) attack on nutritional quality of tomato | 190 |
| PĂTULARU IONUȚ ADRIAN - The “pedagogic” didactic resort ...between idealism and pragmatism | 196 |
| PLOAE MARIETA, DIACONU AURELIA, DIMAMILICA - The influence of climatic factors and technology in some potato varieties grown on sandy soils | 202 |
| PRŽIĆ ZORAN, MARKOVIĆ N. - Influence of partial defoliation and harvest time on ampelographic characteristic of Cabernet Sauvignone grape | 206 |
| PRŽIĆ ZORAN, MARKOVIĆ N., RUML M., VUKOVIĆ A., VUJADINOVIĆ M., RANKOVIĆ-VASIĆ Z. - Variations of climate parameters and their impact on Cabernet Sauvignon and Sauvignon Blanc phenology in conditions of Central Serbia | 214 |
| ROȘCA DANIELA, CSATLOS CAROL, ROȘCA ADRIAN - Considerations on compression strength of tenderized pork meat by using mechanical processing | 221 |
| ROȘCA DANIELA, ROȘCA ADRIAN - The influence of pressuring and vacuuming cyclic process on tenderizing beef pastrami | 232 |
| ROȘCULETE ELENA, ROȘCULETE C.A. - The energy balance for sunflower crops under irrigation and different doses of fertilizers and basic soil operations | 238 |
| SAVESCU PETRE, ANA-MARIADODOCIOIU, CRISTINA MANUELA VLADU, BORUZ SORIN - The development of organic farming in the EU and in Romania- big opportunity for reducing the risks and the hazards that occur in the foods production | 245 |
| SIMIONESCU VIOLETA, MONICA TANC, I. BULICA, DANIELA PLESOIANU - The influence of crop rotation, rotation and fertilization on yield sunflower in climatic conditions from Valul lui Traian | 250 |
| SIMIONESCU VIOLETA, MONICA TANC, I. BULICA, DANIELA PLESOIANU - The long term effect of fertilization on the content of soil micronutrients | 254 |
| SOARE RODICA, NICULESCU MARIANA, PĂNIȚĂ OVIDIU, BONEA DORINA, IANCU PAULA - The biodiversity study of some Rosa canina L. genotypes from Oltenia area | 259 |
| SUMALAN R., DIANA ION, IOANA POPESCU, BRIGITTA SCHMIDT, SUMALAN RENATA, CAMEL D., CIULCA S. - Assessment of phenotypic diversity for some red onion landraces from Timiș County | 264 |
| TOADER MARIA, ROMAN GH. V., ALINA MARIA IONESCU, MIHALACHE M., BĂȘA A.GH., LENUȚA IULIANA EPURE, ION V., DRAKOS A - Competences and job opportunities of organic medicinal and aromatic plants domain developed by Herbal.Mednet project | 270 |
| TRĂSCĂ FLORIAN, IONESCU NICOLAIE, MINCĂ GINA - Study about the lead transfer from sewage sludge into agroecosystems | 275 |
| TRICULESCU MIHAELA - Sustainable agriculture in the Danube valley, Cetate-Dabuleni sector | 281 |
| TRICULESCU MIHAELA - Wetland restoration in Danube Valley, Cetate – Dabuleni sector | 285 |
| VLADU CRISTINA-EMANUELA - Studies on honey authentication and forgery detection | 289 |
| VLADU M., BACILA V., SAVESCU P. - Research on the level of investments, made in the livestock sector, in region of Oltenia, by the National Rural Development Programme 2007-2013..... | 293 |
| GĂVAN CONSTANTIN, MOTORGA VERGIL - Influence of stage and number of lactation on success of the artificial insemination in dairy cows..... | 299 |
| NEȚOIU CONSTANTIN, TOMESCU ROMICĂ, VLADESCU DUMITRU, ALDEA DAN IOAN, BUZATU ANDREI – Evolution of infestations with loopermoth (geometridae) in oak forests from Romania..... | 303 |
| HERNEA CORNELIA, CIRESAN DINU DORIN - Natural regeneration of mixed beech stands | 312 |
| HERNEA CORNELIA, CORNEANU MIHAELA - Phenotypic response of willow cuttings to heavy metals. A preliminary laboratory test | 318 |
| DIHORU GHEORGHE, BORUZ VIOLETA The list of main spontaneous medicinal plants from Romania..... | 324 |
| BORUZ VIOLETA, CRUCERU SONIA - Medicinal plants from greenhouses collection “Al. Buia” Botanical Garden (note II)..... | 341 |

THE CORRELATION STUDIES OF ANTIMYCOBACTERIAL ACTIVITY FOR A NUMBER OF DERIVATIVES OF 4-CARBOXAMIDE

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ABSTRACT

In order to produce a desired physiological effect, substances have to cross cell membranes. The ability of a chemical compound to cross membranes is influenced primarily by the partition coefficient. This is a physical-chemical factor that directly influence the pharmacokinetic profile of the drug and indirect its pharmacodynamic profile. The paper is a QSAR study carried out on a class of substituted of carboxamide, having antimycobacterial activity against the atypical mycobacterial strains and that these compounds are inhibitors of the photosynthesis process. The purpose of such a study is to link the chemical structures of the compounds represented by a set of molecular descriptors with biological activity exhibited by them, expressed as IC₅₀. Identifying these descriptors leads to information of the changes induced by the presence and nature of different chemical groups in the molecule, which allows optimization of analyzed biological activity.

INTRODUCTION

Increasing resistance of tuberculosis to existing currently drugs prompted research antituberculosis into drug development /1-6/.

A study published in this context /7/ report the synthesis and biological activity for a series of carboxylic acid amide derivatives that have been shown to have anti-mycobacterial activity against the atypical mycobacterial strains. Furthermore, these compounds are inhibitors of the photosynthesis process /7/, which may initiate research towards achieving selective herbicides.

In terms of anti-mycobacterial activity, derivatives studied are interesting agents against *Mycobacterium Tuberculosis*, *Mycobacterium Kansasii* și *Mycobacterium Avium*.

In connection with photosynthesis inhibitor activity, it was observed that the activity of some of these compounds inhibit the photosynthesis in chloroplasts.

MATERIALS AND METHODS

As mentioned study is more on chemical synthesis and biological activity experimentally determined, we plan below to perform an QSAR analysis (Quantitative Structure - Activity Relationship) for this class of substances.

The aim is to link the chemical structures of these compounds represented by a set of molecular descriptors with reported biological activity.

The chemical structures of the substances studied are shown in Figure 1.