OVIDIUS UNIVERSITY of CONSTANȚA
Faculty of Applied Sciences and Engineering

Romanian Chemistry Society, Constanța Branch

INTERNATIONAL CONFERENCE "CHIMIA"

BOOK OF ABSTRACTS

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30st of May – 1st of June 2024
Constanța, Romania

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CONFERENCE PROGRAM

Thursday, 30th of May 2024

8^{30} – 9^{30} **Registration**, *Bavaria Blu Hotel, Central Hall*

9^{30} – 9^{50} **Opening ceremony**, *Bavaria Blu Hotel, Conference Room*

Welcome addresses:

- Rector of "Ovidius" University of Constanța
- Conference CHIMIA 2024 Chairperson

9^{50} – 10^{30} **Plenary session (I),** *Bavaria Blu Hotel, Conference Room*

PL1. Andrei MEDVEDOVICI, *University of Bucharest, Romania*

10^{30} – 11^{00} KN1. Nicoleta VÎRVOREA, DOBROGEA GRUP
Consumer chemistry with our products – the magical recipe for success

11^{00} – 11^{20} *Coffee break*

11^{20} – 12^{40} **Plenary session (II),** *Bavaria Blu Hotel, Conference Room*

PL2. Eleonora-Mihaela UNGUREANU, *UNST Politehnica of Bucharest, Romania*

PL3. Timur CHIȘ, *Petroleum - Gas University of Ploiesti, Romania*

12^{40} – 13^{40} **Oral session (I),** *Bavaria Blu Hotel, Conference Room*

13^{40} – 14^{40} *Lunch*

14^{40} – 16^{20} **Oral sessions (II),** *Bavaria Blu Hotel, Conference Room*

16^{20} – 16^{40} *Coffee break*

NOMARES Workshop
New materials for electrochemical recognition of inorganic and biological species

16^{40} – 17^{20} **Plenary session NOMARES Workshop,** *Bavaria Blu Hotel, Conference Room*

PL4. Vesna MIŠKOVIĆ-STANKOVIĆ, *University Union-Nikola Tesla, Belgrade, Serbia*

17^{20} – 17^{40} **Oral session NOMARES Workshop,** *Bavaria Blu Hotel, Conference Room*

17^{40} – 18^{30} **Posters session (I)**, *Bavaria Blu Hotel, Conference Room*

Friday, 31th of May 2024

9^{00} – 11^{00} **Plenary session (III)**, *Bavaria Blu Hotel, Conference Room*

PL5. Stefano GIROTTI, Michele PROTTI, Laura MERCOLINI, Luca FERRARI, *University of Bologna, Italy*

PL6. Cristina Ileana COVALIU-MIERLA, Gigel PARASCHIV, Sorin Stefan BIRIS, *UNST Politehnica of Bucharest, Romania*

PL7. Daniela BERGER, Simona IONITA, Roxana-Cristina POPESCU, Mihaela DEACONU, Mona Mihăilescu, Nicu Tarbă, Cristian MATEI, Liviu CRĂCIUN, Diana-Iulia SAVU, *UNST Politehnica of Bucharest, Romania*

11^{00} – 12^{00} **Oral session (III),** *Bavaria Blu Hotel, Conference Room*

12^{00} – 12^{20} *Coffee break*

12^{20} – 13^{20} **Oral session (IV),** *Bavaria Blu Hotel, Conference Room*

13^{20} - 15^{00} Lunch

15^{00} – 16^{40} **Oral session (V),** *Bavaria Blu Hotel, Conference Room*

16^{40} – 17^{30} **Posters session (II)**, *Bavaria Blu Hotel, Conference Room*

17^{30} – 18^{00} **Closing ceremony**, *Bavaria Blu Hotel, Conference Room*

19^{30} – **Gala Dinner,** *Bavaria Blu Hotel*

Saturday, 1st of June 2024

10^{00} ***Social Program***

The titles of individual presentations in the conference program are hyper-linked to their corresponding abstracts.

For 63 years, our mission has been to enrich consumers' lives with quality, nutritionally balanced products, good consumer care products to be enjoyed any time.

Our mission is to consistently and sustainably grow the Dobrogea brands so appreciated by consumers and to build our business in the global market, through strong brands and strong people and partners.

We are living in a world in which we permanently make choices: from the most basic to very important ones.
In FMCG consumer/shopper choices are done in the store (impulse) or before entering the store in case of a planed shopping.
In pastry category the competition is very high, so shopper choice is either determined by a positive experience that they had before with the product/brand, by crave or by curiosity, the desire to taste something new.
So, the chemistry is not only in the recipe but also in the act of buying and more than that in the re-buying and loyalty.
The permanent focus on the market, consumer trends, economical and social context leads to innovation.
Beside traditional recipes and brand features, there is always the need to differentiate and be flexible and this is the most important challenge: to be chosen from hundred of products and brands at the shelf.

Thursday, 30th of May 2024

$8^{30} – 9^{30}$ **Registration**, *Bavaria Blu Hotel, Central Hall*

$9^{30} – 9^{50}$ **Opening ceremony**, *Bavaria Blu Hotel, Conference Room*

PLENARY LECTURES (I)

$9^{50} – 12^{40}$, Bavaria Blu Hotel, Conference Room

Chairpersons:

Viorica POPESCU, *Ovidius University of Constanta, Romania*
Ionela POPOVICI, *Ovidius University of Constanta, Romania*

PL1. **Andrei MEDVEDOVICI**, *University of Bucharest, Romania*

CURRENT TRENDS IN CHROMATOGRAPHY AND RELATED TECHNOLOGIES

KN1. **Nicoleta VÎRVOREA**, *DOBROGEA GRUP, Romania*

CONSUMER CHEMISTRY WITH OUR PRODUCTS – THE MAGICAL RECIPE FOR SUCCESS

$11^{00} – 11^{20}$ Coffee break

PL2. **Eleonora-Mihaela UNGUREANU**, *UNST Politehnica of Bucharest, Romania*

ON RHODANINE-AZULENE ELECTROCHEMISTRY

PL3. **Timur CHIȘ**, *Petroleum–Gas University of Ploiesti, Romania*

CERTAINTY AND UNCERTAINTY IN PETROLEUM AND PETROCHEMISTRY

ORAL SESSION (I)

12^{40} – 13^{40}, Bavaria Blu Hotel, Conference Room

Chairpersons:

Călin DELEANU, *Center of Organic Chemistry "C.D. Neniţescu" of the Romanian Academy*
Timur CHIȘ, *Petroleum-Gas University of Ploiesti, Romania*

Section A: *Natural and Synthetic Compounds*

OA1. Catalin-Paul CONSTANTIN

ELECTROACTIVE POLYMERS CONTAINING DOUBLE ELECTRON DONOR UNITS WITH POTENTIAL USE IN SMART WINDOW APPLICATIONS

OA2. Robert I. BOTEA, Augustin MĂDĂLAN

STRATEGIC SYNTHESIS OF MONO- AND BINUCLEAR COMPLEXES USING POLYDENTATE LIGANDS WITH EXTENDED π SYSTEMS

OA3. Mihaela DEACONU, Mădălina GHIUȚĂ, Layla ZIKO, Nada SEDKY, Ana-Maria PRELIPCEAN, Ana-Maria SECIU-GRAMA, Ana-Maria BREZOIU, Cristian MATEI, Daniela BERGER

VACCINIUM SP. EXTRACTS ENCAPSULATED IN HOLLOW SILICA SPHERES – ADJUVANTS IN BACTERIAL INFECTIONS

13^{40} – 14^{40} *Lunch*

ORAL SESSION (II)

14^{40} – 16^{20}, *Bavaria Blu Hotel, Conference Room*

Chairpersons:

Gabriela-Iulia DAVID, *University of Bucharest, Romania*
Katya PEYCHEVA, *Medical University of Varna, Bulgaria*

Section A: *Natural and Synthetic Compounds*

OA4. Codruta FRINCUL, Elena BICU, Catalina-Ionica CIOBAN, Sergiu SHOVA, Dalila BELEI

AN EFFICIENT METHOD FOR THE *C*-ALKYLATION OF 1,2,3-TRIAZOLES

OA5. Mădălina-Roxana BIRTEA, Elena BÎCU, Sergiu SHOVA, Dalila BELEI

1,3-DIPOLE CYCLOADDITIONS OF DIMETHYL MALEATE TO N-PHENACYL-4-METHYLPYRIDINIUM BROMIDE

Section B: *Analytical and Environmental Chemistry*

OB1. Laurentiu-Valentin SOROAGA, Cecilia ARSENE, Romeo-Iulian OLARIU

THE INFLUENCE OF COLLISION GAS FLOW AND AEROSOL DILUTION ON THE LOQ OF AN ICP-MS METHOD TAILORED FOR ATMOSPHERIC PARTICLES ANALYSIS

OB2. Silviu-Laurentiu BADEA, Nicolae-Ionut CRISTEA, Violeta-Carolina NICULESCU, Yevheniia KOROLOVA, Costel BUMBAC, Oana-Romina BOTORAN, Roxana-Elena IONETE

BIODEGRADATION OF DIFFERENT HEXACHLORO-CYCLOHEXANE ISOMERS BY *CLOSTRIDRIUM PASTEURIANUM*. STUDY OF KINETICS AND METABOLITES

OB3. Maria-Lorena JINGA, Daniel PREDA, Mihaela DONI, Lucian-Gabriel ZAMFIR, Ana-Maria GURBAN, Gabriela-Iulia DAVID

OPTIMIZATION STUDY FOR INDIRECT VOLTAMMETRIC DETERMINATION OF CORTISOL

16^{20} – 16^{40} *Coffee break*

Workshop *NOMARES*

PLENARY LECTURES (II)

16^{40} – 17^{20} Bavaria Blu Hotel, Conference Room

Chairpersons:

Eleonora-Mihaela UNGUREANU, *UNST Politehnica of Bucharest, Romania*
Gabriela STANCIU, *Ovidius University of Constanta, Romania*

PL4. **Vesna MIŠKOVIĆ-STANKOVIĆ**, *University Union-Nikola Tesla, Belgrade, Serbia*

POLY(VINYL ALCOHOL) HYDROGELS FOR MEDICAL APPLICATIONS

ORAL SESSION NOMARES Workshop

17^{20} – 17^{40}, Bavaria Blu Hotel, Conference Room

ON1. Madalina Marina HRUBARU, Alina VASILE (CORBEI), Amalia STEFANIU, Eleonora-Mihaela UNGUREANU

DENSITY FUNCTIONAL THEORY-BASED ELECTROCHEMICAL MODELS FOR TETRAHYDROACRIDINES

POSTERS (I)

17^{40} – 18^{30}, Bavaria Blu Hotel, Conference Room

Chairpersons:

Andrei MEDVEDOVICI, *University of Bucharest, Romania*
Semaghiul BIRGHILĂ, *Ovidius University of Constanta, Romania*

Section A: *Natural and Synthetic Compounds*

PA1. Ștefania ARDELEANU, Mihaela BADEA, Anca DUMBRAVĂ, Rodica OLAR

SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERISATION OF COPPER(II) COMPLEXES WITH MIXED LIGANDS (AMINO ACIDS AND TRIAZOLOPYRIMIDINE DERIVATIVES)

PA2. Tudor JULA, Cătălin MAXIM, Mihaela BADEA, Anca DUMBRAVĂ, Rodica OLAR

COPPER(II) COMPLEXES WITH N-BASED DONOR LIGANDS DESIGNED AS BIOLOGICALLY ACTIVE SPECIES

PA3. Andra ANDREI, Rodica OLAR, Cătălin MAXIM, Mihaela BADEA

SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERISATION OF COPPER(II) COMPLEXES WITH BENZIMIDAZOLE DERIVATIVES

PA4. Diana AMĂRĂZEANU, Andra ANDREI, Rodica OLAR, Cătălin MAXIM, Mihaela BADEA

SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERISATION OF NEW COMPLEXES WITH PHENANTHROLINE DERIVATIVES

PA5. Ioana-Alexandra TROFIN, Radu-Dan RUSU, Catalin-Paul CONSTANTIN, Mariana-Dana DAMACEANU

FLUORINATED HYPERBRANCHED POLYIMIDES FOR FREE-STANDING MEMBRANES

PA6. Luiza-Mădălina CIMA, Gabriela STANCIU

INVESTIGATION OF THE ANTIOXIDANT PROFILE OF THE WHITE TRUFFLE SPECIES *TUBER MAGNATUM PICO* FROM ROMANIA

PA7. Gabriela STANCIU, Simona LUPȘOR, Elena OANCEA

EVALUATION OF ANTIOXIDANT ACTIVITY IN RELATION TO PHENOLIC CONTENT AND MINERAL PROFILE OF VARIOUS *LILIUM* SPP. BULBS MACERATES

PA8. Gabriela STANCIU, Simona LUPSOR, Ramona ROTARIU

COMPARATIVE STUDY OF THE ANTIOXIDANT ACTIVITY AND MINERAL PROFILE OF ROSEMARY FROM THE AREA OF DOBROGEA AND THE COASTAL AREA OF BULGARIA

Section B: ***Analytical and Environmental Chemistry***

PB1. Alina-Giorgiana NEGRU, Laurentiu-Valentin SOROAGA, Romeo-Iulian OLARIU, Cecilia ARSENE

A COST-EFFECTIVE ICP-MS METHOD FOR TOTAL METALS CONTENT ANALYSIS IN SIZE-RESOLVED ATMOSPHERIC PARTICLES. POTENTIAL HEALTH IMPLICATIONS

PB2. Gabriela Iulia DAVID, Teodora Maria SAVU, Mihaela-Carmen CHEREGI, Emilia-Elena IORGULESCU, Hassan NOOR

SENSITIVE RIFAMPICIN VOLTAMMETRIC DETERMINATION AT THE COST-EFFECTIVE PENCIL GRAPHITE ELECTRODE

PB3. Mihaela-Carmen CHEREGI, Iulia-Gabriela DAVID, Ana-Maria DOBRE, Victor DAVID

VOLTAMMETRIC BEHAVIOR OF TROLOX FOR ESTIMATION OF THE ANTIOXIDANT CAPACITIES OF TOCOPHEROLS IN PHARMACEUTICALS

PB4. Gabriela-Iulia DAVID, George-Eduard FOLTOZAN, Mihaela-Carmen CHEREGI, Emilia-Elena IORGULESCU, Adriana GHEORGHE, Hassan NOOR

LISINOPRIL VOLTAMMETRIC INVESTIGATION

PB5. Gabriela-Iulia DAVID, Adriana GHEORGHE, Mihaela-Carmen CHEREGI, Emilia-Elena IORGULESCU

UV-VIS SPECTROMETRIC ANALYSIS OF BINARY MIXTURES OF BIOLOGICAL AND PHARMACEUTICAL IMPORTANT COMPOUNDS

PB6. Maria Lorena JINGA, Daniel PREDA, Gabriel-Lucian RADU, Petruța OANCEA, Adina RĂDUCAN

THE INFLUENCE OF CAFFEIC ACID IN LACCASE-DIPYRIDAMOLE SYSTEM

PB7. Daniel PREDA, Maria Lorena JINGA, Gabriel-Lucian RADU, Gabriela-Iulia DAVID

DISPOSABLE MIP-BASED ELECTROCHEMICAL SENSOR FOR SENSITIVE DETERMINATION OF DYPIRIDAMOLE

PB8. Daniel PREDA, Anca MATEI, Mihaela-Carmen CHEREGI, Emilia-Elena IORGULESCU,Gabriel-Lucian RADU, Gabriela-Iulia DAVID

OXYTETRACYCLINE ANALYSIS AT DISPOSABLE PENCIL GRAPHITE ELECTRODE

PB9. Ioana-Aspasia BENTOIU (SIMERIA), Cristina ICHIM (VANGHELE), Lucica BARBEȘ

GEOTECHNICAL CHARACTERISTICS OF THE ROMANIAN COASTAL ZONE - INSIGHTS FROM FIELD AND LABORATORY RESEARCH

PB10. Stanislava GEORGIEVA, Angelika GEORGIEVA, Temenuga TRIFONOVA

POLYCYCLIC AROMATIC HYDROCARBONS (PAH) IN BIVALVES (*MYTILUS GALLOPROVINCIALIS*) FROM THE BULGARIAN BLACK SEA COAST AND ASSESSMENT OF POSSIBLE HUMAN HEALTH RISK

PB11. Nicoleta MATEI, Semaghiul BIRGHILA, Simona DOBRINAS, Alina SOCEANU, Viorica POPESCU

METHOD VALIDATION FOR DETERMINATION OF COPPER IN HAIR SAMPLES THROUGH ATOMIC ABSORPTION SPECTROMETRY

PB12. Simona DOBRINAS, Semaghiul BIRGHILA, Nicoleta MATEI, Alina SOCEANU, Viorica POPESCU, Elda CALIL

COMPARATIVE DIGESTION PROCEDURES USED FOR THE DETERMINATION OF Cd, Cr and Pb CONTENT IN BABY FOOD

PB13. Violeta-Carolina NICULESCU, Silviu-Laurentiu BADEA, Laurentiu ASIMOPOLOS, Eugen Laurentiu NICULICI, Violeta-Monica RADU

MAGNETIC BIOCHAR FROM WALNUT SHELLS MODIFIED WITH CATIONIC SURFACTANT

PB14. Nicoleta MATEI, Semaghiul BURGHILA, Simona DOBRINAS, Alina SOCEANU, Viorica POPESCU, Roxana PRICOPIE

QUALITY EVALUATION OF EDIBLE OILS AVAILABLE IN ROMANIAN LOCAL MARKET

PB15. Maria COVEI, Dana PERNIU, Cristina BOGATU, Camelia DRAGHICI, Anca DRAGHICI

EDUCATIONAL INITIATIVES TO FACE PLANETARY BOUNDARIES CAUSED BY PLASTIC RELEASE IN ENVIRONMENT

PB16. Maria COVEI, Cristina BOGATU, Dana PERNIU, Ioana TISMANAR, Anca DUTA, Hermine STROESCU, Madalina NICOLESCU, Jose Maria CALDERON MORENO, Irina ATKINSON, Mariuca GARTNER

VIS-ACTIVE PHOTOCATALYTIC THIN FILM BEADS FOR WASTEWATER TREATMENT

PB17. Gabriel DOBRICĂ, Naliana LUPAȘCU, Carmen MAFTEI, Ionela CARAZEANU POPOVICI

CURRENT CHEMISTRY OF NUNTASI LAKE AND ITS TEMPORAL CHANGES

Section C: *Physical Chemistry*

PC1. Mihaela SILION, Daniela IONITA, Mariana CRISTEA

STRUCTURAL INVESTIGATIONS OF POLYESTER RESINS WITH ANTHRACENE-PROTECTED MALEIMIDE GROUPS USING MASS SPECTROMETRY AND THERMAL ANALYSES

PC2. Aycan ALTUN KAVAKLI, Osman Nuri ŞARA, Mioara-Jeanina LUNGU, Sibel OSMAN

THERMOPHYSICAL AND EXCESS PROPERTIES OF BINARY BLENDS OF BIODIESEL WITH DIETHYL ETHER, DIETHYLENE GLYCOL DIMETHYL ETHER AND DIMETHYL CARBONATE AT DIFFERENT TEMPERATURES

NOMARES Workshop

PN1. Irinela CHILIBON, Ovidiu-Teodor MATICA, Cristina VASILIU, Gabriela STANCIU, Elena DIACU, Eleonora-Mihaela UNGUREANU

STUDY OF SENSITIVE ELECTRODES BASED ON COMPLEXING AZULENE POLYMER FILMS

PN2. Elena Valentina IONITA, Alina Giorgiana BROTEA, Ovidiu-Teodor MATICA, Magdalena-Rodica BUJDUVEANU, Francis Aurelien NGOUNOUE KAMGA, Eleonora-Mihaela UNGUREANU

OPTICAL AND ELECTROCHEMICAL EXPERIMENTS FOR Hg(II) ANALYSIS IN SOLUTION AND ON AZULENE-PHENYLOXAZOLONE-CMEs

PN3. Maria-Francesca TICULESCU, Anastasia BURLACIOC, Madalina-Marina HRUBARU, Francis Aurelien NGOUNOUE KAMGA, Elena DIACU, Eleonora-Mihaela UNGUREANU

CHEMICALY MODIFIED ELECTRODES BASED ON SEVERAL AZULENYL-PHENYLOXAZOLONE FOR Cu(II) ANALYSIS

PN4. Cecilia LETE, Mariana MARIN, Sorina Alexandra LEAU, Stelian LUPU

DEVELOPMENT OF SENSITIVE NANOCOMPOSITE MATERIALS FOR BIOLOGICALLY ACTIVE COMPOUNDS

PN5. Amalia STEFANIU, Alina-Giorgiana BROTEA, Ovidiu-Teodor MATICA, Oana ENACHE, Gabriela STANCIU, Eleonora-Mihaela UNGUREANU

OPTICAL EXPERIMENTS AND DFT CALCULATIONS FOR AZULENE-PHENYLOXAZOLONES

PN6. Cornelia Elena MUȘINĂ (BORȘARU), Alina-Giorgiana BROTEA, Madalina PANDELE, Roxana TRUSCA, Mihaela CRISTEA, Eleonora-Mihaela UNGUREANU

MODIFIED ELECTRODES BASED ON ETHENE-2,1-DIYLTETRATHIOPHENE AZULENE DERIVATIVE FOR HEAVY METALS ANALYSIS

PN7. Andreea DRĂGOI BRÎNZA, Raluca Ioana VAN STADEN, Damaris Cristina GHEORGHE, Gabriela STANCIU

DETERMINATION OF EICOSAPENTANOIC ACID ETHYL ESTER IN THE LIVER OF STINGRAY

PN8. Andreea-Elena DORNEANU, Raluca-Ioana VAN STADEN, Catalina CIOATES NEGUT, Gabriela STANCIU

DETERMINATION OF HUMIC ACID IN SAPROPEL USING A NEW STOCHASTIC SENSOR

Friday, 31th of May 2024

PLENARY LECTURES (III)

9^{00}– 11^{00}, Bavaria Blu Hotel, Conference Room

Chairpersons:

Cristina BOGATU, *Transilvania University of Brasov, Romania*
Mihaela CHEREGI, *University of Bucharest, Romania*

PL5. **Stefano GIROTTI, Michele PROTTI, Laura MERCOLINI, Luca FERRARI**

NEW PSYCHOACTIVE SUBSTANCES (NPS): EDUCATION AND RISK PREVENTION THROUGH INNOVATIVE PEDAGOGICAL MODELS FOR STUDENTS

PL6. **Cristina Ileana COVALIU-MIERLA, Gigel PARASCHIV, Sorin Stefan BIRIS**

CURRENT APPLICATION OF NANOTEHNOLOGY IN WASTEWATER TREATMENT

PL7. **Daniela BERGER, Simona IONITA, Roxana-Cristina POPESCU, Mihaela DEACONU, Mona Mihăilescu, Nicu Tarbă, Cristian MATEI, Liviu CRĂCIUN, Diana-Iulia SAVU**

DRUG DELIVERY SYSTEMS BASED ON FUNCTIONALIZED MESOPOROUS SILICA FOR CANCER THERAPY

ORAL SESSION (III)

11^{00} -12^{00} *Bavaria Blu Hotel, Conference Room*

Chairpersons:

Daniela BERGER, *UNST Politehnica of Bucharest, Romania*
Anca DUMBRAVĂ, *Ovidius University of Constanta, Romania*

Section C: *Physical Chemistry*

OC1. Adriana-Petronela CHIRIAC, Catalin Paul CONSTANTIN, Mariana Dana DAMACEANU

POLYMER BLENDS BASED ON POLYIMIDES CONTAINING TRITYL-SUBSTITUTED TRIPHENYLAMINE FOR CO_2 SEPARATION MEMBRANES

OC2. Andra-Elena BEJAN, Catalin-Paul CONSTANTIN, Mariana-Dana DAMACEAN

TRIPHENYLMETHANE BASED-POLYIMIDES: SYNTHESIS AND CHARACTERIZATION

OC3 Mihaela SILION, Cristina M. AL-MATARNEH, Razvan Cristian PUF, Mariana PINTEALA

MASS SPECTROMETRIC CONFIRMATIONS REGARDING MECHANISTIC INSIGHTS IN THE DOEBNER REACTION

12^{00} – 12^{20} Coffee break

ORAL SESSION (IV)

12^{20} -13^{20} *Bavaria Blu Hotel, Conference Room*

Chairpersons:

Stefano GIROTTI, *University of Bologna, Italy*
Timur CHIS, *Petroleum - Gas University of Ploiesti, Romania*

Section D: *Petroleum Technology and Management*

OD1. Ioana-Alexandra TROFIN, Radu-Dan RUSU, Catalin-Paul CONSTANTIN, Mariana-Dana DĂMĂCEANU

THIOPHENE BASED HYPERBRANCHED POLYMERS FOR ELECTROCHROMIC AND ENERGY STORAGE APPLICATIONS

OD2. Claudia Ana Maria PATRICHI, Doinita Roxana CIOROIU TIRPAN, Ali A. Abbas ALJANABI, Bogdan TRIC, Ioana Catalina GIFU, Tanase DOBRE

EXTRACTION OF CELLULOSE FROM ULVA LACTUCA ALGAE AND ITS USE FOR MEMBRANE SYNTHESIS

Section E: *Food Chemistry and Engineering*

OE1. Cătălin DUDUIANU, Raluca STAN, Alina NICOLESCU, Calin DELEANU

NMR METABOLOMICS OF TOMATOES DEGRADATION

13^{20} -15^{00} Lunch

ORAL SESSION (V)

15^{00} -16^{40} *Bavaria Blu Hotel, Conference Room*

Chairpersons:

Veselina PANAYOTOVA, *Medical University of Varna, Bulgaria*
Ancaelena Eliza STERPU, *Ovidius University of Constanta, Romania*

Section F: *Medicinal and Pharmaceutical Chemistry*

OF1. Anca Daniela RAICIU, Amalia STEFANIU

ACTIVE COMPOUNDS IN GLYCERIN HYDROALCOHOLIC EXTRACTS WITH POTENTIAL ANTI-INFLAMMATORY EFFECT

OF2. Anca Daniela RAICIU, Amalia STEFANIU

PLANT EXTRACTS RICH IN NATURAL POLYPHENOLS AND FLAVONOIDS WITH LIVER-PROTECTIVE EFFECTS

OF3. Cristina Maria AL-MATARNEH

UNLOCKING THE ANTIMICROBIAL POTENTIAL OF SMALL NITROGEN MOLECULES

OF4. Ramona LUNGU, Daniela AILINCAI, Luminita MARIN

AN EXPERIMENTAL STUDY ON CHITOSAN-BASED HYDROGELS BIODEGRADATION FOR WOUND HEALING

OF5. Calin DELEANU, Cătălin DUDUIANU, Alina NICOLESCU

NMR LIPIDOMICS

POSTERS (II)

16^{40}- 17^{30}, Bavaria Blu Hotel, Conference Room

Chairpersons:

Andrei MEDVEDOVICI, *University of Bucharest, Romania*
Semaghiul BIRGHILĂ, *Ovidius University of Constanta, Romania*

Section D: *Petroleum Technology and Management*

PD1. Adriana-Petronela CHIRIAC, Mariana Dana DAMACEANU

CONJUGATED POLYMERS BASED ON THIOPHENE FOR USE AS ELECTROCHROMIC AND CAPACITIVE MATERIALS

PD2. Andra-Elena BEJAN, Catalin-Paul CONSTANTIN, Mariana-Dana DAMACEANU

NON-CONJUGATED ProDOT-BASED POLYAMIDES FOR ELECTROCHROMIC CAPACITIVE WINDOWS

PD3. Sorin-Lucian IONAȘCU, Lucica BARBEȘ

RECYCLING AND VALORIZATION OF COMPONENTS FROM END-OF-LIFE VEHICLES THROUGH ADVANCED AND SUSTAINABLE TECHNOLOGIES

PD4. Emanoil-Andrei POPA, Viorel IONESCU, Anisoara - Arleziana NEAGU

PERFORMANCE EVALUATION OF A THERMOELECTRIC COOLING BOX SYSTEM

PD5. Stefania PIRVU, Viorel IONESCU, Anisoara - Arleziana NEAGU

ONE-DIMENSIONAL THERMAL MODEL FOR TEMPERATURE EVALUATION INSIDE THE WATER – COOLED PEMFC

PD6. Andrei BĂRBULESCU, Laura Andrea SFIRIAC, Maria STOICESCU

OPTIMISATION OF OIL PRODUCTION FUNCTION TO POROUS ROCKS

PD7 Doru BÂRSAN, Dan Ovidiu CIRJAN, Maria STOICESCU

TREATMENT OF HYDROCARBON-POLLUTED WATERS THROUGH OXYGEN AND OZONE NANOBUBBLE TECHNOLOGY

PD8 Doru BÂRSAN, Timur CHIS

SEPARATION OF WATER FROM NATURAL GASES

PD9 Mihaela HELSTERN, Laura Andrea SFIRIAC, Maria STOICESCU

REZERVOIR OPTIMISATION OF OIL PRODUCTION BY IPR CURVES

PD10 George Tiberiu SANDU, Claudiu DOLETTE, Maria STOICESCU

OPTIMISATION OF GAS STORAGE

PD11 George Tiberiu SANDU, Timur CHIS

THE EFFECT OF CO_2 ON COLLECTOR ROCKS IN OIL FIELDS

PD12 Alla ZEINAB, Andrei BĂRBULESCU1, Timur CHIS

EFECTS OF ACID TO OIL ROCKS

PD13 Daniel IANCU, Al Jaseem Ameer MAKI, Timur CHIS

CORROSION IN ROMANIAN OIL PLATFORMS - A CASE STUDY

PD14 Daniel IANCU, Al Jaseem Ameer MAKI, Timur CHIS

ODORIZATION OF NATURAL GAS- A CASE STUDY

PD15 Derya UNLU, Sibel OSMAN

A COMPARATIVE STUDY ON APPLICATION PROPERTIES OF DIESEL FUEL BLENDS WITH DIBUTYL ETHER (DBE)

PD16 Ancaelena Eliza STERPU, Olga Valerica SAPUNARU

EFFICIENT AND ECOLOGICAL PROCESSES IN OBTAINING SOAPS FROM WASTE COOKING OILS

PD17 Ancaelena Eliza STERPU, Olga Valerica SAPUNARU

UTILIZING WASTE COOKING OIL AS LUBRICATING OIL: A SUSTAINABLE APPROACH TO AUTOMOTIVE MAINTENANCE

PD18 Mihaela HELSTERN, Timur CHIS

MODELING POLYMER MOVEMENT IN RESERVOIR ROCKS

Section E: ***Food Chemistry and Engineering***

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PLENARY LECTURES

PL1. CURRENT TRENDS IN CHROMATOGRAPHY AND RELATED TECHNOLOGIES

Andrei MEDVEDOVICI

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Since the official birth date of chromatography in 1906, it seems that almost nothing has changed, at least considering its basic principles. However, the technique takes benefits from the major advances of the technology and the accumulation of knowledge in the related fields of analytical chemistry. What happens new in chromatography and the related technologies after 120 years of maturation? Four directions should be followed indeed: 1. Instrumentation; 2. Column technology and stationary phase; 3. Mobile phase composition; 4. Alternatives in sample preparation & sample transfer.

The major achievements in instrumentation mainly focused on the detecting systems. The basic Flame Ionization Detector (FID) for gas chromatography was upgraded with a catalytic reactor leading to the QCD-FID (Quantitative Carbon Detector) in order to produce proportional response with respect to the carbon content of the detected analytes. The spectrometric UV detector shifted from liquid chromatography (LC) to gas chromatography (GC), leading to Vacuum UV (or Far UV) detector. For compensation, the FTIR detector from GC moved to LC, using a transfer interface quite similar to former technical solutions used in the late '80s for making agreement between LC and Mass Spectrometry (MS). Molecular Rotational Resonance Spectroscopy (MRRS) based on a Fourier Transform (FT) platform, having intrinsic structural confirmation ability combined with isotope indicating characteristics will become commercially available in the very near future. Selected Ion Flow Tube Mass Spectrometry (SFIT-MS), due to its ability to control the ionization stage, also emerges as an interesting alternative for GC detection, through adding selectivity. Last but not least, Ion Mobility Spectrometry (IMS), known as gas phase electrophoresis, being in fact a separation technique, is nowadays commercially available in at least eight working modes variants. IMS is actually used as a second dimension in 2-D separations (the first dimension is GC or LC) and may be easily hyphenated with the MS detection.

Trends in column technologies and stationary phase chemistry brought into attention the micropillar arrays for micro and nano-LC, the stationary phase gradients and the bimodal behavior of the new born stationary phases.

New findings about mobile phase composition in LC refers to the use of green organic solvents as alternatives for the classic ACN/MeOH modifiers. Another direction (is this a fashion?) deals with the use of ionic liquids as additives (chaotropic agents) in Reversed Phase LC applications.

Quite recent aspects related to sample preparation for LC involve the use of Supramolecular Solvents (SUPRAS) in extraction processes and the ability of achieving Large Volume Injection (LVI) with sample diluents not miscible with the mobile phase.

PL2. ON RHODANINE-AZULENE ELECTROCHEMISTRY

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Electrochemical characterization of several rhodanine-azulenes was performed by cyclic voltammetry, differential pulse voltammetry, and rotating disk electrode voltammetry to establish the common features and particularities of these structures. Parallel studies on for heavy metal (HM) ions complexation in solution were done by UV-Vis.

Taking into account the fact that azulene compounds require special conditions for the synthesis, the analogy between azulene derivatives of rhodanine and dialkylaminobenzylidene rhodanine creates the premises for an easier selection of azulene compounds with interesting properties for a certain application. Comparison of the electrochemical studies of these compounds revealed the similarity between the electrochemical processes of oxidation and reduction, which confirmed the similarity of the chemical properties of the two compounds, which is expected considering the similar electron-donating character of these structures [1, 2].

However, preparation of modified electrodes based on various rhodanine-azulenes and their electrochemical characterization to be used for Pb ions analysis revealed the superiority of azulene based monomer [3]. Evidence for films formation by scanning and controlled potential electrolysis was furnished, and HMs recognition experiments using their films were carried on. The performance of the chemically modified electrodes was evaluated as detection limits for HMs. The azulene monomer which proved to be the best candidate for Pb(II) detection was found about ten times more sensitive than the other rhodanine derivatives.

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PL3. CERTAINTY AND UNCERTAINTY IN PETROLEUM AND PETROCHEMISTRY

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The oil and petrochemical industry has ensured the economic growth and material well-being of millions of people around the globe for the last 100 years. Without black gold components, industrial activity would not occur at current development standards.

Throughout history, the control of petrochemical processes has developed in parallel with the application of knowledge from mathematics and physics in this field.

If, in the first stage of the petrochemical industry, the control of technological processes was done by reading and writing in notebooks the operating data and was based on the knowledge and especially on the skill of the supervisors to operate the processes, today it is not conceived as the reading of the parameters, the transfer of these data and processing for numerical operation not to be done with the help of high-speed computers.

Unfortunately, the data collected, processed, and treated necessary for the automatic control of petrochemical processes led to the reading and storage of over 1,000,000 operating parameters (pressures, temperatures, densities, viscosities, concentrations, etc.) per day.

All these parameters must be analyzed and integrated into complex numerical models, and artificial intelligence is becoming increasingly necessary.

That is precisely why this material presents the techniques for processing operating data of petrochemical plants in the context of artificial intelligence, especially anti-virus protection systems.

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PL4. POLY(VINYL ALCOHOL) HYDROGELS FOR MEDICAL APPLICATIONS

Vesna MIŠKOVIĆ-STANKOVIĆ

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The biomaterials field is always evolving towards finding new wound dressing formulations which can provide active protection of the wound from bacterial infections. Hydrogel-based materials are especially interesting for such a purpose, considering their favorable biocompatibility, sorption and mechanical properties, as well as the potential for immobilization and incorporation of antibacterial agents. The synthesis of silver nanoparticles (AgNPs) became very interesting for potential applications in biomedicine, since nanocrystalline silver is proved to be the most efficient antimicrobial agent with a wide inhibiting spectrum towards different types of microorganisms. AgNPs embedded in hydrogel matrices are attractive for biomedical applications due to possibility for their controlled release resulting in antimicrobial activity. Thus, combination of AgNPs with biocompatible hydrogels, poly(vinyl alcohol) (PVA) and chitosan (CHI), provides potential for design of improved medical treatments. Graphene (Gr) has exceptional mechanical properties and has therefore been applied as adequate reinforcing component for composite materials. In this work, we synthesized new composite hydrogels with electrochemically synthesized silver nanoparticles, Ag/PVA/Gr and Ag/PVA/CHI/Gr, aimed for wound dressing materials. Hydrogels were characterized by UV-Vis, CV, FE-SEM, Raman, AAS, FT-IR, MTT cytotoxicity tests and test of antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*. The results indicated that both hydrogels are excellent candidates for soft tissue implants and wound dressings [1-3].

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PL5. NEW PSYCHOACTIVE SUBSTANCES (NPS): EDUCATION AND RISK PREVENTION THROUGH INNOVATIVE PEDAGOGICAL MODELS FOR STUDENTS

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New Psychoactive Substances (NPS) are a growing group of chemical compounds with dangerous toxicological properties, posing significant health risks. According to the European Drug Report [1], addressing NPS diffusion represents a public health challenge. Approximately 5% of young people aged 15 to 24 in Europe have consumed NPS [2], with a higher prevalence among minors. The project "Innovative teaching and learning paths for the prevention of new drug abuse" (INES, ines.unibo.it) aims to increase education and prevention activities by sharing expertise among stakeholders; implement sustainable teaching activities in school curricula; empower teachers and students and support innovation at the school system level [3]; involve stakeholders in defining and implementing strategies to address NPS; exploit participative working models to incorporate gaming into teaching-learning processes; design the curriculum to engage students and empower teachers. INES project, coordinated by Alma Mater Studiorum - University of Bologna (Erasmus+ KA2, grant 2021-1-IT02-KA220-SCH-000032570), involves academic partners and secondary schools in Romania, Portugal and Italy. The project focuses on creating conditions to support collaborative networking among teachers, experts and students to develop and test teaching strategies to address NPS issues. Outputs include a European syllabus on NPS, an online course, a game prototype and a pedagogical planner for teachers.

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PL6. CURRENT APPLICATION OF NANOTEHNOLOGY IN WASTEWATER TREATMENT

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Water containing pollutants such as organic and inorganic compounds, pathogens, or other toxins, making it unsafe for the ecosystem, is called to as wastewater.

Industries worldwide have implemented various schemes to treat wastewater before releasing it back into the environment. Traditional methods are being rapidly replaced by innovative concepts and technologies [1-5]. This article provides a brief overview of recent advances and applications of nanotechnology in wastewater treatment. Nanomaterials, with their high reactivity, extensive functionalization, large specific surface area, and size-dependent properties, are particularly suitable for wastewater treatment. The article discusses the use of various nanomaterials, including metal nanoparticles, metal oxides, carbon compounds, zeolites, and filtration membranes, in the context of wastewater treatment. Also, will be presented some high wastewater efficiencies (> 90%) obtained for removing inorganic (heavy metals) and organic (dyes, fats and drugs) pollutants through adsorption, oxidation and flotation processes.

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PL7. DRUG DELIVERY SYSTEMS BASED ON FUNCTIONALIZED MESOPOROUS SILICA FOR CANCER THERAPY

Daniela BERGER,[1] Simona IONITA,[1] Roxana-Cristina POPESCU,[2] Mihaela DEACONU,[1] Mona MIHĂILESCU,[3] Nicu TARBĂ,[3] Cristian MATEI,[1] Liviu CRĂCIUN,[2] and Diana-Iulia SAVU[2]

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Efficient cancer treatment usually involves combined therapies, which include surgery, radiation treatment, chemotherapy, etc. Patients can receive a favorable radiation treatment after surgery, with or without chemotherapy, such as neutron, proton, photon, ion, boron proton-capture enhanced proton (BPCEPT) therapies, which involves the use of a beam positioning in such a way to achieve the mean adsorbed dose in the tumor area [1]. On the other hand, because chemotherapy is widely used for cancer treatment, the design of efficient targeted drug delivery systems that decrease the harmful effects on normal tissues represents an approach with many benefits for patients' health. Mesoporous silica nanoparticles (MSN) are widely applied as carriers in drug delivery systems due to their ability to accommodate a tailored amount of biologically active molecules with tuned interactions with carrier's surface depending on functionalization [2]. In this regard, we use for the design of novel targeted drug delivery systems, MSN functionalized with phenylboronic acid moieties (MSN-BA) that bind on sialic acid receptors overexpressed by breast cancer cells and can also be useful for BPCEPT. Herein, we report our results on doxorubicin and/or resveratrol delivery from MSN-BA in PBS pH 5.5. Best results regarding the antitumoral effects on BT474 breast cancer cells were obtained for co-delivery system. The internalization rate of samples in cancer cells investigated by hyperspectral microscopy, evidenced the highest rate when cytostatic agent was loaded on MSN-BA.

Acknowledgements: *The authors are grateful to UEFISCDI for the financial support though PED576/2022 project.*

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SECTION A: NATURAL AND SYNTHETIC COMPOUNDS

OA1. ELECTROACTIVE POLYMERS CONTAINING DOUBLE ELECTRON DONOR UNITS WITH POTENTIAL USE IN SMART WINDOW APPLICATIONS

Catalin-Paul CONSTANTIN

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As part of our pursuit of new advanced materials capable of tackling current technological concerns, we developed the chemical blocks to build new polymers viable as electrochromic (EC) energy storage materials. In this context and inspired by our prior research [1], this study introduces a novel strategy for developing fresh electroactive POZ-based materials to be integrated into electrochromic energy storage (EES) devices. For this purpose, a new structural designed diamine with a pendant double electron-donor core by attaching POZ to a diphenylamine (DPA) structure was conceived and synthesized. This structural approach was used to augment primarily the electrochemical stability and solubility enhancement of the proposed materials. Then, to test the "power" of the diamine's POZ–DPA-based core, three polymeric platforms were used, including a polyimide (PI), a polyazomethine (PAz) and a polyamide (PA). Through this approach, we endeavored to ascertain the superior performer among these three distinct categories of polymers with respect to their electrochemical and electrochromic characteristics. The correct chemical structure of all synthesized organic compounds was confirmed by common spectroscopy tools, followed by a complete physico-chemical and computational evaluation. Subsequently, the POZ–DPA-based polymer exhibiting the most favorable electrochemical and EC characteristics in the three-electrode cell setup was selected for further assessment. This involved the construction of laboratory-scale EES prototype devices to evaluate their performance with regard to both EC and energy storage efficiency and stability so that the full applicative potential to be unlocked.

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OA2. STRATEGIC SYNTHESIS OF MONO- AND BINUCLEAR COMPLEXES USING POLYDENTATE LIGANDS WITH EXTENDED π SYSTEMS

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The development of polydentate imino and amino ligands has led to significant advancements in the design of homo- and heteropolynuclear complexes that contain 3d and 4f metal ions. These ligands, with multiple binding sites, offer greater stability and a diverse range of structural possibilities for the formation of complex structures. In the synthesis of such complexes, a stepwise approach is commonly employed, where the 3d ion is introduced first, followed by utilizing the resulting complex as a ligand towards the 4f ion.

In this study, a series of innovative polydentate Schiff base ligands were synthesized, utilizing *N*-(1-naphthyl)ethylenediamine and various phenol aldehydes. These imino ligands and the amino derivatives obtained by reduction were used either alone or in combination with other chelatic ligands to generate both mono- and binuclear complexes. X-ray diffraction on single crystals was employed to structurally characterize the ligands and complexes, revealing the versatility of these imino and amino derivatives as bidentate, tridentate, or tetradentate ligands.

Furthermore, the study analyzed the optical properties of the synthesized ligands and complexes in the solid-state through IR, UV-Vis, and luminescence spectroscopy. These analyses provide insights into the electronic and structural properties of the ligands and complexes, which are crucial for understanding their potential applications in other fields of chemistry.

OA3. *VACCINIUM SP.* EXTRACTS ENCAPSULATED IN HOLLOW SILICA SPHERES – ADJUVANTS IN BACTERIAL INFECTIONS

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Plant extracts have been proven to possess antimicrobial activity, but their minimum inhibitory concentration is usually significantly larger than that of conventional antimicrobial agents, making it highly improbable to be used as a substitute for antibiotics. However, in the struggle against resistant microorganisms, plant extracts could be used as adjuvants in conventional antibiotic therapy. In this study, phytochemicals with antibacterial properties were extracted from plant leaves from *Vaccinium* genus: lingonberry (*Vaccinium vitis idea*) and wild bilberry (*Vaccinium myrtillus*), both plants that have been long used in traditional medicine. Lingonberry leaves and stems are used to relieve discomfort in urinary tract infections or inflammations, and wild bilberry leaves and stems support the digestive system and assist in glucose metabolic process. The properties of these extracts were assessed (radical scavenger activity, total polyphenols content, total flavonoids content, total tannins content, antidiabetic activity) and the components of these extracts were identified through HPLC. After carefully assessing these properties, the extracts with the greatest potential for developing a pharmaceutical formulation were chosen to be encapsulated in hollow silica spheres, thus providing an aid in infection treatment plan.

Acknowledgements: *This work was performed during PCE 117/2022 project which was founded by UEFISCDI.*

OA4. AN EFFICIENT METHOD FOR THE C-ALKYLATION OF 1,2,3-TRIAZOLES

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The 1,2,3-triazole nucleus has attracted considerable attention in recent decades due to its multiple biological activities. This heterocyclic structure has become a focal point in medicinal chemistry and related fields due to its non-toxic nature and stability under biological conditions [1].

To investigate the impact of the substituent at the 4-position of 2-(4-(hydroxymethyl)-*1H*-1,2,3-triazol-1-yl)-1-phenylethan-1-one, the functionalization of the oxygen atom in the hydroxymethyl group by its alkylation was considered. To this end, a large number of experiments were carried out with different inorganic and organic bases, using ethyl bromoacetate as the alkylating agent. The results obtained revealed competition between the reactivity of the methylene group in position 1 of the 1,2,3-triazole ring and the -OH group of the hydroxymethyl radical.

In none of the experiments, O-alkylating compounds were isolated. Elimination compounds containing the 1,2,3-triazole skeleton substituted in the 1-position with the radical from ethyl bromoacetate were identified in low yields. To ensure the certainty and accuracy of the results, all newly synthesized compounds were subjected to rigorous purification and characterized in detail both physically and spectroscopically. The structure of the obtained derivative was confirmed by single-crystal XRD.

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OA5. 1,3-DIPOLE CYCLOADDITIONS OF DIMETHYL MALEATE TO *N*-PHENACYL-4-METHYLPYRIDINIUM BROMIDE

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The interest in heterocyclic nitrogen compounds has increased over the past century due to their properties [1]. The synthesis of these heterocyclic derivatives can be achieved by various methods, one of them being the 1, 3-dipole cycloaddition reaction, which offers the possibility of obtaining compounds with well-determined structures and stereochemistry [2].

N-phenacyl-4-methylpyridinium bromide is successfully used as a dipole 1,3 generator in these cycloaddition reactions using dipolarophiles with both symmetrical and non-symmetrical structures [3], thus obtaining heterocyclic derivatives with indolizin structures.

Dimethyl maleate has been used as dipolarophile in previous studies, where the dipole 1,3 was generated from *N*-phenacyl-*N,N*-dimethylaminopyridinium bromide, reaction from which were unexpectedly isolated bis-lactonic compounds of the Pechamnn dye class.

The mechanism of the elimination reaction by which bis-lactonic structures are obtained is elucidated, as well as the aspects related to the mechanism of the double cycloaddition reaction, a concurrent reaction to that of elimination in the presented system are clarified, through which adducts with tri- respectively tetracyclic structures are obtained [4].

The present study uses *N*-phenacyl-4-methylpyridinium bromide as a precursor of dipole 1,3 and no studies have been reported so far on its conversion to bislactonic and tricyclic compounds in the presence of dimethyl maleate. The dipole 1,3 was generated in the presence of triethylamine and reaction products were chromatographically purified and analyzed by IR, ^{1}H-NMR and ^{13}C-NMR.

Acknowledgements: *The authors thank the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for recording the NMR spectra.*

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PA1. SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERISATION OF COPPER(II) COMPLEXES WITH MIXED LIGANDS (AMINO ACIDS AND TRIAZOLOPYRIMIDINE DERIVATIVES)

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The copper ion is an essential ion involved in several biological processes' regulation. Its stereochemical and oxidation state versatility, acid borderline character, and lower systemic toxicity are features that recommend this ion for the synthesis of complexes with a large variety of ligands, structures and properties [1].

As result, many copper complexes with antitumor, anti-inflammatory or antimicrobial activity were designed. Most of these complexes contain mixed ligands, one being a N-O-chelating heterocycle such an amino acid, chosen both for its chelating ability and intercalative properties. Hence, several Cu(II) complexes with this kind of ligands were synthesized and some known as Casiopeínas® evidenced a very good antitumor potential based on a nuclease like activity [2].

Having in view these aspects, we extended this field in synthesis of new series of complexes of type $[Cu(His)_2(tp)]$ and $[Cu(His)_n(tp)_m](ClO_4)$ (n and m 1 or 2; Hhis: histidine and tp: 5,7-dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine (dmtp) or 5-methyl-7-phenil-1,2,4-triazolo[1,5-*a*]pyrimidine (mftp)) with tp as auxiliary ligand. The features of complexes have been assigned from elemental analyses as well as IR, and UV-Vis spectra. The tp ligands behave as unidentate while histidine acts as chelate. A distorted square pyramidal or tetrahedral stereochemistry is completed by perchlorate as free ions.

The complexes will be tested for both antimicrobial and antitumor activities.

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PA2. COPPER(II) COMPLEXES WITH N-BASED DONOR LIGANDS DESIGNED AS BIOLOGICALLY ACTIVE SPECIES

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The essential biocation copper is usually involved in biologically active complexes design based on its lower systemic toxicity. This is accompanied by other useful properties such stereochemical and oxidation state versatility, and acid borderline character, that allows interaction with a wide range of target biomolecules [1].

As result, several copper complexes that exhibit antitumor, anti-inflammatory or antimicrobial activity were reported. Most of these species are based on ligands with both chelating ability and intercalative properties such as N-heterocycles derived from pyridine and triazolopyrimidine [2].

In order to modulate biological activity, we extended this field in the synthesis of new series of complexes of type $[Cu(N\text{-}N)_2(tp)](ClO_4)_2$ (N-N = 2,2'-bipyridine and 1,10-phenantroline and tp = 5,7-dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine). The compounds were characterized based on data provided by elemental analyses, IR, and UV-Vis spectra as well as single crystal X-ray diffraction. The tp ligand behaves as unidentate while N-N ones act as chelate in a distorted square pyramidal stereochemistry.

The complexes will be tested for both antimicrobial and antitumor activities.

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PA3. SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERISATION OF COPPER(II) COMPLEXES WITH BENZIMIDAZOLE DERIVATIVES

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In recent years, significant progress has been made in designing new antineoplastic drugs containing benzimidazole-type ligands coordinated with transition metals from the 3d, 4d, and 5d series in their structure. Results published in various studies have demonstrated that elements from the *d*-block can be used as potential anticancer drugs in combination with benzimidazole, as they can interact with cellular structures, especially with DNA, thus inducing lesions and cell death through various mechanisms of action.

Studies have demonstrated that the majority of complex combinations exhibit significantly better activity than that of the free ligand. Therefore, coordinating the metal ion to the benzimidazole ligand has a remarkable effect on cytotoxic activity, as the resulting compound intervenes in the polarity balance, favoring its penetration through the lipid layer of the cell membrane.

Four new complex combinations of copper (II) with benzimidazole derivatives as ligands have been synthesized: $[Cu(2\text{-}MeBzim)_2(Macr)_2]$, $[Cu(5\text{-}MeBzim)_2(Macr)_2]$, $[Cu(5,6\text{-}Me_2Bzim)_2(Macr)_2]$ and $[Cu_2(2\text{-}MeBzim)_2(Macr)_4]$ (2-MeBzim = 2-methylbenzimidazole, 5-MeBzim = 5-methylbenzimidazole, 5,6-Me_2Bzim = 5,6-dimethylbenzimidazole, Macr = metacrylate anion). These have been characterized through elemental chemical analysis, thermal analysis, electronic and IR spectroscopy, as well as X-ray diffraction. The combinations differ in nuclearity, the stereochemistry of the metal ion, and the mode of coordination of the methacrylate anion.

The complexes will be tested for both antimicrobial and antitumor activities.

PA4. SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERISATION OF NEW COMPLEXES WITH PHENANTHROLINE DERIVATIVES

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The new generations of metal-based chemotherapeutics have provided a fresh perspective on combating cancer on a global scale, increasing the number of cancer types that can be treated. Keratocyte carcinomas (KCs) and localized cutaneous melanomas offer a distinct opportunity for the development of topical treatments based on metallotherapeutics [1].

The metal complexes possess some properties like ionic nature, adjustable polarity and the ability to act as pro-drugs which could lead to their use as drugs for topical treatments.

In the end, metallotherapeutics can be customized to regulate their ability to penetrate the skin, offering crucial approaches for treating localized skin conditions. Additionally, they present an opportunity to reach systemic levels, when necessary, which is particularly crucial for managing invasive melanomas [2].

Four new complex combinations of copper (II) and nickel (II) with 1,10-phenanthroline/4,7-diphenil-1,10-phenanthroline as ligands have been synthesized: $[Mphen(Macr)_2(H_2O)]$, (M: Cu, Ni), $[CuPh_2phen(Macr)_2]$, and $[Ni_2(Ph_2phen)_2(Macr)_4(H_2O)]DMF$ (phen = 1,10-phenanthroline, Ph_2phen = 4,7-diphenil-1,10-phenanthroline, Macr = metacrylate anion). These have been characterized using elemental chemical analysis, thermal analysis, electronic and IR spectroscopy, as well as X-ray diffraction.

The complexes will be tested for antitumor activities.

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PA5. FLUORINATED HYPERBRANCHED POLYIMIDES FOR FREE-STANDING MEMBRANES

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Hyperbranched polymers are a new class of three-dimensional macromolecules being recognized by unique properties derived from the large number of terminal units that come with the cost of laborious synthesis protocol, limited control over molar mass and over branching points [1]. Hyperbranched polyimides are considered high-performance polymers well-distinguished for thermal and dielectric properties, and also improved solubility compared to their linear analogues. Also, the presence of the generous free volume determined by the molecular geometry implies an intrinsic microporosity well desired for gas-separation membranes [2].

This work aimed at design, synthesis and optimization of a series of fluorinated hyperbranched polyimide architectures that can generate free-standing membranes [3]. The primary goal was to identify the ideal ratio between monomers bearing different functionalities to be used in the polymer synthesis as to attain superior solubility and processability, as well as desired physico-chemical characteristics of the polymers. Thus, optical performance, dielectric behavior, thermal resistance, and outstanding morphology relevant for intrinsic microporosity of the polymers were highlighted in relation with their further applications in gas separation membranes. In addition, new strategies for preventing the gelation in synthesis of hyperbranched polyimides are discussed.

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PA6. INVESTIGATION OF THE ANTIOXIDANT PROFILE OF THE WHITE TRUFFLE SPECIES *TUBER MAGNATUM PICO* FROM ROMANIA

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Continuing research within the scientific community is focused on exploring the many benefits of antioxidant compounds, in particular their anti-aging and anti-inflammatory properties [1]. Recognition of the value of antioxidants in the food industry has led to their successful integration into a wide range of products, increasing their nutritional content and effectively addressing potential problems.

Romanian truffles, like all truffles, are highly searched for their unique taste and nutritional value [2]. However, the chemical composition of these prized mushrooms is strongly influenced by the specific conditions in which they grow [3]. Although there have been numerous studies examining the phytoconstituents found in different truffle species, research on Romanian truffles remains limited. The most commercially significant truffle species, known as the white truffle (*Tuber magnatum Pico*), is highly valued for its sensory attributes and restricted geographical area. Therefore, the objective of this study is to identify the specific compounds responsible for the antioxidant effects found in truffles, including the total phenol and flavonoid content, and to evaluate the antioxidant properties (DPPH method) of four macerates obtained from truffles using different solvents.

Four white truffle macerates were obtained using different solvents, mainly deionized water (TA), 70% ethyl alcohol (TE70), 96% ethyl alcohol (TE96) and methanol (TM), all in a 1:5 ratio of truffle to solvent. These four macerates were analyzed spectrophotometrically to determine their total phenol content (TPC) using the Folin-Ciocâlteau method and total flavonoid content (TFC) according to FR.X, in accordance with the monograph for "*Cynarae folium*".

Flavonoids have the ability to absorb UV radiation, playing a vital role in protecting the body against the harmful effects of oxidative stress and free radicals, which have the potential to cause cell damage. The extraction of flavonoids yielded the most significant results when using TM and TA macerates, with 396.41 mg rutin/100 g truffle for TM and 302.34 mg rutin/100 g truffle for TA. On the other hand, the macerates utilizing alcoholic

and hydroalcoholic solvents produced the lowest concentrations. This discovery indicates that the selection of solvent plays a crucial role in determining the levels of flavonoid extraction [4]. In terms of TPC analysis, the results obtained from all four macerates were similar.

Following the analysis for total antioxidant capacity by DPPH method, it was found that macerates from the white truffle *Tuber magnatum Pico* show remarkable antioxidant capacity. This antioxidant activity is predominant in all samples that were analyzed. Sample TM showed the highest level of antioxidant capacity at 88.91% while sample TE96 showed the lowest level of DPPH radical scavenging capacity at 23.15%.

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PA7. EVALUATION OF ANTIOXIDANT ACTIVITY IN RELATION TO PHENOLIC CONTENT AND MINERAL PROFILE OF VARIOUS *LILIUM* SPP. BULBS MACERATES

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Lilium species have been reported to contain bioactive compounds such as polyphenolic compounds including alkaloids, flavonoids, sterols, saponins, vitamins, organic acids and minerals, making them promising candidates for therapeutic applications.[1, 2] Concentrations of these compounds vary by species, variety and growing conditions. Experimental studies on various *Lilium* species indicate significant potential for antioxidant, anti-inflammatory and antimicrobial properties. [3, 4]

Ten macerate samples from five distinct cultivars of *Lilium* spp. bulbs were analyzed in this study. Alcoholic maceration was employed using two types of solvents: S1, consisting of 98% ethanol, and S2, containing ethanol with a concentration of 75%.

The Folin-Ciocâlteau method was used for the evaluation of total phenolic compounds. The findings showed that *Lilium* bulb macerates showed high concentrations of phenolic compounds, ranging from 122.76 to 295.48 mg GAE/100 g f.w.

The quantification of total flavonoid content by the sodium nitrite method for the evaluation of flavonoid levels in the analyzed samples was expressed as quercetin equivalent (mg QE/100g f.w.), showing a close similarity with the values reported in the literature for the analyzed samples.

Antioxidant capacities were evaluated using the DPPH Radical Scavenging assay, revealing significant antioxidant activity in the tested samples.

Metal concentrations were assessed using the AAS method, revealing substantial levels of K, Na and Ca, along with the presence of Mg and Fe in the analyzed samples. In addition, traces of Zn, Cu, Mn, Cr and Ni were detected, while concentrations of Pb and Cd fell below detection limits.

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PA8. COMPARATIVE STUDY OF THE ANTIOXIDANT ACTIVITY AND MINERAL PROFILE OF ROSEMARY FROM THE AREA OF DOBROGEA AND THE COASTAL AREA OF BULGARIA

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Rosemary (*Rosmarinus officinalis*) is a versatile herb valued for its culinary and medicinal properties, rich in phenolic compounds like carnosic acid, carnosol, and rosmarinic acid [1, 2]. Rosemary's versatility extends across culinary, traditional medicinal, and emerging therapeutic domains, including cancer prevention and cognitive health. Comparative analysis of rosemary from diverse geographic regions provides valuable insights for its potential applications across various fields [3].

For this study, six macerates were prepared using sources from both Dobrogea and the Bulgarian coastal region. Each sample underwent maceration in three different solvents: ethanol solutions with concentrations of 40%, 70%, and 96%, all under controlled conditions.

The Folin-Ciocâlteau method was employed to analyze the samples and quantify total phenolic compounds. Findings revealed that macerates derived from rosemary in the Bulgarian coastal region exhibit higher concentrations of phenolic compounds compared to those from the Dobrogea region. Additionally, 70% alcohol was identified as the most effective solvent.

Antioxidant activity was assessed using the DPPH Radical Scavenging test, revealing that the analyzed samples demonstrated significant antioxidant potency between 107.50 mg GAE/100g f.w. (from Dobrogea coastal region samples) and 103.5 mg GAE/100g f.w. (from Bulgarian coastal region samples). Metal concentrations were assessed using the AAS method, revealing significant levels of Ca, Na, K, Mg, and Fe, with lower concentrations of Cu, Mn, Zn, Cr, and Ni. Pb and Cd concentrations were below the detection limits.

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SECTION B: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

OB1. THE INFLUENCE OF COLLISION GAS FLOW AND AEROSOL DILUTION ON THE LOQ OF AN ICP-MS METHOD TAILORED FOR ATMOSPHERIC PARTICLES ANALYSIS

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The ICP-MS technique is characterized by sensitivity at sub-ppb level of concentration, making it suitable for metal content determination from atmospheric particles [1]. However, the quadrupole mass filter is prone to isobaric, polyatomic, and doubly-charged interferences due to its limited resolution. The contribution of the interferents to the analyte signal can be reduced, if not totally removed, by optimizing a series of parameters, but this can also have a negative effect on the performance of the measurements, in terms of sensitivity [2].

In this study, the impact on the limit of quantification (LoQ) of the collision gas flow and the use of aerosol dilution, together with some other parameters, was evaluated. The internal standard calibration (with ^{45}Sc, ^{89}Y and ^{159}Tb) was performed from 0.1 µg l^{-1} to 50 µg l^{-1} for B, Mg, Al, Cr, Mn, Co, Ni, Cu, Zn, Ga, Sr, Ag, Cd, Ba, Tl, and Pb. Both aerosol dilution and no aerosol dilution analysis modes have been used, with collision gas flow (He) of 0 / 80 / 120 ml min^{-1}. It was found that while some parameters have little to low influence on the sensitivity, others must be fine-tuned regarding the sample matrix in order to obtain the best sensitivity while maintaining the interferences on a low level.

The optimized method was used for the analysis of NIST 1649b – Urban dust CRM and the determined concentrations have been found to be in good agreement with the certified values of concentration.

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OB2. BIODEGRADATION OF DIFFERENT HEXACHLOROCYCLOHEXANE ISOMERS BY *CLOSTRIDRIUM PASTEURIANUM*. STUDY OF KINETICS AND METABOLITES

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In this study, to mimic the anaerobic biodegradation of HCHs at contaminated sites occurring through reductive dehalogenation, the biodegradation of γ-HCH and δ-HCH isomers by *Clostridrium pasteurianum* DSM 525 has been investigated. Degradation experiments with *C. pasteurianum* were performed in 1 L bottles crimped gas-tight with Teflon-coated butyl septa. In both experiments, the sterile medium (500 mL) was spiked from stock solutions of acetone (about 400 mM for γ-HCH and 3.43 mM for δ-HCH, respectively) to a final concentrations of 20-21.5 µM, not exceeding their solubility limit in water of about 24-34 µM [1]. A set of culture bottles was inoculated with 10–20 mL of *C. pasterurianum* preculture and continuously shaken for two hours at 150–200 rpm, while a second set was kept sterile to act as a control. The bottles were incubated up to 15 days at 30 °C with 125 rpm stirring speed set on the incubator. At regular intervals, 14 mL of aqueous solution was taken from the bottles using plastic syringes for extraction, and this was then extracted with 1 mL dichloromethane (DCM) containing 107 µM hexachlorobenzene (HCB) and 103 µM toluene as internal standards. For δ-HCH experiment, the GC-MS/MS analyses were performed using a 1310 Trace series GC gas chromatograph coupled with a TSQ 8000 EVO triple quadrupole mass spectrometer (Thermo Fisher Scientific, Germany) configured in Scan mode. In the control bottle, the concentration of δ-HCH decreased from 24.1 µM at the beginning of the experiment to 20.5 µM after 15 days, indicating no significant degradation. In the culture flask inoculated with *C. pasteurianum*, the concentration of δ-HCH varied from 24.3 µM at the start of the experiment to 17.9 µM after 15 days, indicating a limited biodegradation of δ-HCH by *C. pasteurianum*. Consequently, additional investigations are warranted to elucidate the kinetics and degradation pathway of δ-HCH and γ-HCH by *C. pasteurianum*.

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OB3. OPTIMIZATION STUDY FOR INDIRECT VOLTAMMETRIC DETERMINATION OF CORTISOL

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Cortisol is a hormone with special significance for the body's survival due to its role in regulating key functions like blood pressure, heart rate and stress responses, playing an important role in immune, metabolic and homeostatic processes. Given its importance, there is a need for the development of simple and reliable methods for rapid cortisol detection in various biological samples. This work reports the development of an indirect voltammetric method for cortisol determination using a molecularly imprinted polyproflavine modified pencil graphite electrodes (MIP_PGE).

Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) studies showed that cortisol is electrochemically inactive and its direct determination is not possible. Thus, an indirect approach was realized based on the decrease in the oxidation signal of $[Fe(CN)_6]^{4-/3-}$ in the presence of cortisol. Higher anodic signals of the redox probe and their significant decrease in the presence of the analyte were observed at the MIP_PGE. The modified electrodes were characterized by Scanning Electron Microscopy (SEM). In order to achieve a highly sensitive determination of cortisol, an optimization of several parameters, such as electropolymerization solutions (acetate, phosphate and NaOH supporting electrolytes), extraction time and solvent of cortisol from MIP, and the incubation time of electrodes in cortisol varying from 0 to 30 minutes, was performed.

Further studies aim to establish the performance characteristics of the MIP_PGE (linear range, limits of detection and quantification, selectivity) and its application to the cortisol determination in real samples (e.g. saliva).

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PB1. A COST-EFFECTIVE ICP-MS METHOD FOR TOTAL METALS CONTENT ANALYSIS IN SIZE-RESOLVED ATMOSPHERIC PARTICLES. POTENTIAL HEALTH IMPLICATIONS

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In the atmospheric particulate matter evaluation, the elemental composition is of utmost importance due to various elements negative effects on human health [1]. When correlated with the size of particles, this jointed approach provides a substantially more comprehensive image of the negative impact associated with the investigated site [2].

In this study, the total elemental composition of size-resolved atmospheric particles collected from Iasi, North-Eastern Romania, was evaluated by using a high sensitivity ICP-MS from the Analytik Jena PlasmaQuant MS Series (Elite). The samples were collected on aluminum filters at the Air Quality Monitoring Station (AMOS) in Iasi, using a 13-stage cascade Dekati Low-Pressure Impactor (DLPI) with average particles size between 0.0276 µm and 9.94 µm. The sample dissolution was performed by microwave-assisted wet digestion with HNO_3 65%, followed by a minimum dilution with ultrapure water prior analysis. The internal standard (^{115}In) multi-element calibration was preferred. For selected metals (e.g., Bi, Cd, Co, Mn, Pb, Zn) the results were evaluated in terms of their mass concentration distribution by size. Health risk was also evaluated for potential toxic elements and the results were compared with other studies.

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PB2. SENSITIVE RIFAMPICIN VOLTAMMETRIC DETERMINATION AT THE COST-EFFECTIVE PENCIL GRAPHITE ELECTRODE

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Rifampicin (RIF) is a macrocyclic broad-spectrum antibiotic activ agains a large variety of bacteria and eukaryotes [1]. It is still the main medicine used to prevent or treat tuberculosis. Due to the fact that RIF presents concentration-dependent toxicity and possible drug resistance, as well as its possible leakage in the environment, leading to persistent toxicity and distortion in the ecosystems, its reliable and simple quantification in various samples is very important. From chemical point of view, RIF is a hydroquinone derivative bearing three phenolic −OH groups which can be chemically or electrochemically oxidized. Therefore, herein we present RIF voltammetric analysis at the cost-effective, disposable pencil graphite electrode (PGE).

Differential pulse voltammetry (DPV) studies performed at different working electrodes pointed out that the RIF oxidation signal presented the highest sensitivity at HB type PGE. Cyclic voltammetric (CV) studies indicated that RIF presents a cvasi-reversible peak pair corresponding to the quinone-hydroquinone redox couple. From the different dependencies of the peak currents on the scan rate applied in CV, one can conclude that RIF electrode processes were adsorption controlled. CV and DPV investigations indicated that RIF oxidation was pH-dependent and involved an equal number of electrons and protons. The highest RIF DPV signals were obtained at pH 1.81. Their currents varied linearly with the analyte concentration in the range $7.50 \times 10^{-8} – 1.00 \times 10^{-6}$ M RIF and $5.00 \times 10^{-8} – 1.00 \times 10^{-6}$ M RIF for the anodic and the cathodic peaks, respectively. The corresponding detection limits were 1.80×10^{-8} M and 2.55×10^{-8} M RIF.

PB3. VOLTAMMETRIC BEHAVIOR OF TROLOX FOR ESTIMATION OF THE ANTIOXIDANT CAPACITIES OF TOCOPHEROLS IN PHARMACEUTICALS

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Trolox (6-hydroxy-2,5,7,8-tetramethylchromane-2-carboxylic acid) (TX) is a naturally occurring lipid soluble antioxidant and the most active component of vitamin E, analogue of α-tocopherol (α-TOH) [1]. In the chemical structure of TX, the hydrocarbon chain from position 2 of α-TOH is replaced by a carboxyl group, which lead to a more hydrophilic character than α-TOH and its antioxidant properties are attributed to the ability of hydroxyl group, from position 6, to interact with free radicals. TX is most widely used to assess the antioxidant capacity of various products, and the analytical method using TX is called the *Trolox equivalent antioxidant capacity* (TEAC) assay. This work presents the voltammetric behavior of TX and its use for the estimation of the antioxidant capacity of two different commercially available α-TOH containing pharmaceutical products (multivitamin tablets and children syrup).

The TX electrochemical properties were studied in aqueous media using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). CV was performed to select the best conditions for TX electrochemical determination, such as: the working electrode (vs. Ag/AgCl); the electrolyte solution; the scan rate and pH influence on the anodic peak intensity ($I_{p,ox}$). The best TX voltammetric results were obtained on glassy carbon electrode (GCE) when a TX characteristic anodic peak was observed around 0.340 V in CV and, respectively, 0.270 V in DPV using as supporting electrolyte, Britton Robinson buffer, pH = 4. Under the optimized experimental conditions, the $I_{p,ox}$ values measured in DPV, were linearly dependent on TX concentration in the range of 5–200 μM. This voltammetric approach was applied to assess the antioxidant capacity of two tocopherols containing pharmaceutical products, expressed as *mg equiv. TX / product*.

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PB4. LISINOPRIL VOLTAMMETRIC INVESTIGATION

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Lisinopril (LP) is an angetionsin-converting enzyme inhibitor employed in the hypertionsion medication treatment. Very often LP is used in combination with hydrochlorthiazide (HCT), a diuretic from the thiazide group. Therefore, there is a need for new simple and reliable methods for the rapid determination of LP in the presence of HCT, from different matrices. The present work deals with the voltammetric investigation of LP at a disposable pencil graphite electrode (PGE) and its quantification in the presence of HCT.

Differential pulse voltammetry (DPV) studies emphasized that the highest and best defined LP oxidation signal was obtained at inactivated HB type PGE using phosphate buffer solution (PBS) pH 7.00 as supporting electrolyte. Britton Robinson buffer (BRB) solutions with pH values in the range 2.21 – 11.58 were used to investigate the influence of pH on LP anodic peak, which increased and shifted towards more negative potentials when the solution pH changed from 2.21 to 7.96. The slope of the regression equation describing the E_p = f(pH) dependence indicated that LP electrooxidation involved an equal number of electrons and protons. According to the cyclic voltammetric results, this process was diffusion controlled. Using the above mentioned optimized conditions LP, was quantified by both DPV and square wave voltammetry (SWV) within the linear ranges 2.50×10^{-5} – 2.50×10^{-3} M and 5.00×10^{-5} – 1.00×10^{-3} M LP, respectively. The corresponding attained detection limits were $2{,}00 \times 10^{-6}$ M and 7.57×10^{-6} M LP.

Unfortunately, using DPV and SWV at PGE under the above mentioned conditions, LP could not be detected in the presence of HCT but it was possible by using BRB pH 11.92, when in the presence of 1.00×10^{-4} M HCT, the linear range for LP determination was 2.50×10^{-4} – 2.50×10^{-3} M LP for both voltemmetric methods. The developed DPV and SWV methods were applied to LP quantification in pharmaceutical preparations.

PB5. UV-VIS SPECTROMETRIC ANALYSIS OF BINARY MIXTURES OF BIOLOGICAL AND PHARMACEUTICAL IMPORTANT COMPOUNDS

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UV-VIS spectrometric methods are simple and do not need expensive instrumentation but, unfortunately, they lack on selectivity. However, this performance characteristic can be improved by either derivatization, which involves reagents and supplementary time and special conditions, or by applying the "green" alternative represented by derivative spectrometry.

The present work discusses a comparative study of simultaneous spectrometric determination of species commonly found together in various samples, by using the absorbance additivity law and the first and second order derivative spectrometry. The selected pairs of analytes were: the polyphenolic acids: gallic acid (GA) and ellagic acid (EA), the bioflavonoids: hesperidin (HESP) and diosmin (DIO) and the drugs sulphamethoxasole (SMX) and trimethoprim (TMP). The optimum analysis conditions were established by monitoring the effect of pH on the absorption spectrum of each analyte, recorded in Britton-Robinson buffers (BRB) with different pH-values comprised in the range 1.81-11.58. Using the optimized conditions, the practical applicability of the methods was tested by quantification of the analytes from pharmaceuticals (for SMX and TMP in BRB pH 11.58 and for HESP and DIO in BRB pH 6.80) and from dietary supplements (GA and EA in BRB pH 1.81). The DIO and HESP contents of pharmaceuticals were also determined with good results by the H-point standard addition method.

PB6. THE INFLUENCE OF CAFFEIC ACID IN LACCASE-DIPYRIDAMOLE SYSTEM

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Laccases (LAC) isolated from *Trametes versicolor* are enzymes commonly used in dye industry as bleaching agents. Another use can be found in pulp delignification and whitening industry where degrades all phenolic compounds found in lignin. The degradation of phenolic compounds requires a laccase - mediator systems. Interestingly, no kinetic model has been found in the literature to describe the mediator effect during the phenolics decomposition. Caffeic acid (CA) is a phenolic compound synthesized by all plant species and is present in foods such as coffee, wine, tea, and popular medicines such as propolis. This phenolic acid and its derivatives have antioxidant, anti-inflammatory and anticarcinogenic activity. The aim of this study is to determine the influence of caffeic acid as a mediator for the degradation of dipyridamole in the presence of laccase.

We studied the influence of the substrate (DYP) in laccase reaction using a spectrophotometric determination. The conversion of the substrate was followed at 400 nm. From this we obtained the Michaelis-Menten parameters, K_M and V_{max}. The influence of pH was also studied, ranging between 3.00 - 8.00. The highest enzyme activity was found at pH 4.40. From the variation of the enzyme concentration, we determined the inactivation constant using an isoconversional method. A reaction mechanism was proposed considering the rates in the global process. We studied the importance of caffeic acid as a mediator resulting that the degradation of the dipyridamole is enhanced by a small quantity of mediator.

The understating of the reaction mechanism it is not well achieved, but studying the influence of different mediators helps degrading faster the pharmaceuticals found in unpleasant places.

PB7. DISPOSABLE MIP-BASED ELECTROCHEMICAL SENSOR FOR SENSITIVE DETERMINATION OF DYPIRIDAMOLE

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Dipyridamole (DYP) is one of the most prescribed antithrombotic drugs administered orally. Its use was limited due to side effects such as coronary ischemia, headaches and abdominal pain. Even though its negative effects have been demonstrated, this did not stop athletes from using it for doping purposes such as reducing fatigue and improving sports performance. Curcumin (CUR) is a widely researched and utilized natural product known for its antioxidant activity and its capacity to reduce the oxidative stress. Due to its phenolic groups, CUR is electrooxidized while the formed phenoxy radicals polymerize. The aim of the this study was to develop an inexpensive, efficient, sensitive and selective DYP-imprinted poly(CUR) modified sensor in order to determine DYP from different matrices.

The polymerization process was performed at non-activated HB type PGE using NaOH as supporting electrolyte. The polymerization conditions were optimized with respect to the CUR:DYP ratio, pH of the polymerization solution, number of polymerization cycles and scan rate in voltammetric deposition. The optimum extraction time in ethanol for complete removal of the template molecule from the polymeric matrix was also established. The influence of pH on DYP determination was studied, the best defined and highest signal being obtained at pH 2.21. DYP was quantified by differential pulse voltammetry (DPV) within the linear ranges 5.00×10^{-8} – 1.00×10^{-5} mol/L and 2.50×10^{-5} – 1.00×10^{-4} mol/L DYP, respectively. Applying the adsorptive stripping voltammetric (Ads-DPV) technique under the optimized accumulation conditions at MIP_PGE a linear range between 5.00×10^{-9} to 1.00×10^{-7} mol/L DYP was obtained.

The disposable MIP_PGE modified sensor can be used to determine the concentration of DYP in tablets and tap water.

PB8. OXYTETRACYCLINE ANALYSIS AT DISPOSABLE PENCIL GRAPHITE ELECTRODE

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Oxytetracycline (OTC) is a wide-spectrum antibiotic belonging to the tetracycline class. It is used in human and veterinary medicine for the treatment of various bacterial infections and also as feed additive for animals [1]. Uncontrolled consumption of OTC can result drug accumulation in animal food products, as well as in environmental, leading to growth of antibiotic-resistant bacteria, the antibiotic becoming thus inactive against this microorganisms. Therefore, there is an increased need in the development of simple, rapid and reliable methods for OTC determination in various matrices. This work presents OTC voltammetric analysis at the disposable, cheap pencil graphite electrode (PGE).

OTC electrochemical response investigated at different types of working electrodes emphasized that the highest sensitivity was exhibited by PGE using HB type pencil leads. Electrochemical pretreatment of the PGE did not bring any improvement in OTC oxidation signal. The influence of the solution pH on OTC was investigated in the range 2-11, by both cyclic (CV) and differential pulse voltammetry (DPV) in Britton-Robinson Buffer (BRB). OTC irreversible, diffusion controlled oxidation was pH-dependent involving an equal number of electrons and protons. The highest signal was recorded at pH 4.56.

Applying DPV at PGE OTC oxidation peak increased linearly with the analyte concentration in the range 1.00×10^{-6} to 3.60×10^{-4} mol × L^{-1}. The method's limit of detection was calculated to be 6.80×10^{-7} mol × L^{-1} OTC. The applicability of the developed DPV method using PGE was tested by OTC quantification in pharmaceutical preparations. Employing the standard addition method, the obtained recovery was 103.12%.

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PB9. GEOTECHNICAL CHARACTERISTICS OF THE ROMANIAN COASTAL ZONE - INSIGHTS FROM FIELD AND LABORATORY RESEARCH

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A geotechnical study was conducted from 2020 to 2022 to reduce the risks of erosion and flooding in the Black Sea coastal area. The primary objective was to determine the foundation conditions by assessing the physico-chemical and mechanical characteristics of the terrain at the Tomis Nord site. Samples collected from the site through geotechnical drilling (which included eight standard dynamic penetration tests) were analyzed for granulometry and $CaCO_3$ content [1-2]. The laboratory analyses followed internal protocols using the Scheibler method for determining $CaCO_3$ content and the granulometric method, along with microscopic analysis for determining shell fragment content. Samples from shore surveys indicated a high average content of shell fragments (53.78% w/w) and $CaCO_3$ (74.71% w/w) compared to samples from offshore surveys, which showed a lower average content of shell fragments (17.55% w/w) and $CaCO_3$ (31.79% w/w). Based on the results, it was found that the stratification on the shore consists of loose sand down to a level of -2.3 m, a layer of cohesive clay materials between -2.3 m and -7.7 m, and degraded limestone rock below -7.7 m. The offshore stratification consists of loose silty sand down to a depth of 1.5 m, a layer of sandy clay between 1.5 m and 3 m, and the base rock of degraded limestone starting from 3 m depth. The study results classify the terrain as difficult ground, necessitating urgent rehabilitation work [3].

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PB10. POLYCYCLIC AROMATIC HYDROCARBONS (PAH) IN BIVALVES (*MYTILUS GALLOPROVINCIALIS*) FROM THE BULGARIAN BLACK SEA COAST AND ASSESSMENT OF POSSIBLE HUMAN HEALTH RISK

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The polycyclic aromatic hydrocarbons (PAHs) were classified by International Agency for Research on Cancer (IARC) as probable or possible human carcinogens and they are able to cause mutagenic effects in humans and others animal species [1]. The aim of the study was to assess the present contamination levels of PAHs in black mussel (*Mytilus galloprovincialis*) and to estimate the potential health risks associated with seafood consumption. The wild and farmed mussels were collected from different sampling areas of the Bulgarian Black Sea coast in the period winter 2021 – spring 2022. The concentrations of 13 individual PAH compounds in mussel soft tissues were determined by extraction in accelerated solvent extractor (ASE) and were detected by gas chromatography system with mass spectrometry detection (GC-MS).

The results showed the prevalence of phenanthrene and fluorene as the most abundant compounds in all mussel samples. Although benzo[a]pyrene was detected in 33% of analyzed samples, the concentrations did not exceed the limit set in EC Regulation. The low molecular weight (LMW) PAHs (3 and 4 aromatic rings) were predominant accounting 96.5% of total PAH levels in mussels investigated. The ratio LMW/HMW PAHs was higher than one, suggesting pollution predominantly of petrogenic origin. The sum of four priority PAH (4PAHs) in *Mytilus galloprovincialis* from Sozopol (southern area) was found higher (0.72 ng/g ww) than Northern sampling point (Kavarna) - 0.33 ng/g ww. The sum of 4 PAHs (mean 0.35 ng/g ww) in mussels from Black Sea coast of Bulgaria was found below legislation limit. The potential health risk was assessed using daily intake of PAHs and hazard quotient (HQ) and showed that that shellfish consumption did not pose a risk to human health.

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PB11. METHOD VALIDATION FOR DETERMINATION OF COPPER IN HAIR SAMPLES THROUGH ATOMIC ABSORPTION SPECTROMETRY

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A simple, cheap, and sensitive analytical method was validated for the determination of copper in human hair after microwave digestion. Method validation parameters such as linearity, precision, accuracy, limit of detection (LOD) and limit of quantification (LOQ) were determined. A graphite furnace - atomic absorption spectrophotometer has been used. The developed method was linear in the concentration range of 0.002 - 0.020 μg/mL with a 0.9979 coefficient of determination. The recoveries obtained for the copper ranged from 90.5-95.3%, with a precision not exceeding 1.58% relative standard deviation. LOD was found to be 0.0017 mg/L and LOQ 0.0058 mg/L. The analyzed samples were from healthy humans and the study shown similar concentration of copper in hairs collected from men, women, and children. The proposed method was considerate adequate for the determination of copper in hair samples.

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PB12. COMPARATIVE DIGESTION PROCEDURES USED FOR THE DETERMINATION OF Cd, Cr AND Pb CONTENT IN BABY FOOD

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This study compared the dry ashing, microwave, and wet digestion methods of processing baby food samples for Cd, Cr and Pb analysis. The concentrations of studied heavy metals were determined in varieties of baby food samples with fruits, vegetables, cereals, and meat, obtained from Constanta, Romania. A graphite furnace - atomic absorption spectrophotometer has been used for the analysis of Cd, Cr and Pb concentration in baby foods. The results showed significant differences in the data obtained after processing with the three digestion methods. The microwave method showed lower standard deviation for Cd, Cr and Pb determination in baby food samples. The concentrations of Cr and Pb in baby food samples were in the range of 0.58-2.72; 1.01-5.23 mg/kg, respectively. Cd was detected only in three samples in the range of 0.05-0.23 mg/kg. The maximum permissible limits for children are 0.02 mg/kg Pb in infant formulae and 0.2 mg/kg Pb in cereals and vegetables, while for Cd is 0.05 mg/kg in fruits and vegetables and 0.1 mg/kg in cereals. From the obtained data it can be observed that most of the samples exceed the maximum permissible limits.

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PB13. MAGNETIC BIOCHAR FROM WALNUT SHELLS MODIFIED WITH CATIONIC SURFACTANT

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The walnut shells represent major refuse in the worldwide fruits and nuts market. This waste must be discarded, a solution being its carbonization to biochar - a value-added product with various applications such as adsorbent or catalytic support. These applications are imposed by structural and chemical modification of the resulted biochar. In this study, biochar was prepared by pyrolysis at 550 °C from walnut shells as raw material. Magnetic biochar with high adsorption capacity was further treated with 1M $FeCl_3$, followed by calcination at 550 °C. To overpass a well-known problem of powder adsorbent (difficulty to separate them from the solution), a functionalization of the magnetic biochar was performed using cetyltrimethylammonium bromide (CTAB). The final products were characterized by FTIR, SEM, Raman, AAS, elemental and magnetic analysis. The biochar presented irregular shaped particles of bulk carbon structures. Elemental and EDS analysis showed that the samples were mainly composed of carbon, iron, oxygen, chlorine, calcium, and potassium. Still, iron content decreased after biochar modification with by CTAB. The magnetic biochar proved to have ferromagnetic behavior with the magnetic remanence to saturation magnetization ratio of less than 25%. Further studies will investigate the biochar adsorption properties for different dyes found in wastewater.

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PB14. QUALITY EVALUATION OF EDIBLE OILS AVAILABLE IN ROMANIA LOCAL MARKET

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The aim of the study was to analyze and understand the physico-chemical quality indices of edible vegetable oils used for cooking purpose in Romania. The results will help us for selecting a good quality edible oil. Eight types of oils were selected in this project which are: sunflower, ultra-virgin and organic olives, grape seeds, rapeseed, walnuts, rice and a mixture of flax, rapeseed, pumpkin. Different analytical procedures like measuring the total phenolic activity of oils, iodine numbers, saponification number of oils, peroxide index, acidity, and some metals determinations were performed on all categories of oils. Heavy metals levels (cadmium, lead, copper, chromium, cobalt, nickel and manganese) were assessed using graphite furnace atomic absorption spectrometry (GF-AAS).

No large differences were found between the measured concentrations of the studied heavy metals. The content of heavy metals in extra virgin olive oil were within the limits of the values found in extra virgin oil from Spain (1 ppm Mn and Cu, 3.3 ppm Cr, 1.5 ppm Cd, 2.6 ppm Pb, 0.5 ppm Co, 1.3 ppm Ni). The highest amount of Cr and Cu was found in rapeseed oil, Mn and Co in walnut oil, Pb in rice oil, Ni in grape seed oil and Cd in extra virgin olive oil.

The concentrations of total polyphenols in the studied oils are between 1.40 and 50.62 mgGAE/100 g, the lower values being recorded in sunflower oil. Physico-chemicals quality indices, acidity, peroxide index, the iodine numbers, and the saponification numbers, with small deviations, characterize the oils studied as qualitative oils and allowed to be used in food. The iodine index is lower than the usual average, for all types of oil, which indicates a low amount of unsaturated fatty acids, while the saponification index values indicate a good quality of the oils. These analyses are carried out to ensure that the vegetable oil is safe to use, is not adulterated and does not contain harmful substances.

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PB15. EDUCATIONAL INITIATIVES TO FACE PLANETARY BOUNDARIES CAUSED BY PLASTIC RELEASE IN ENVIRONMENT

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During last century, among the new chemicals and products developed to increase the humanity wellbeing, plastics emerged as versatile, durable, not expensive, actually ubiquitous materials. Nowadays it is known their negative impact on the environment all over their lifecycle, from raw material to the waste phase. It has been demonstrated that fossil-based plastics, assumed as novel entities have already transgressed the planetary boundaries, having high effects on biodiversity loss, climate change, ocean acidification. The drastic environmental damages emphasis the urgent need of transforming our behaviors. It is at planetary level, where decisions and changes are strongly related to policies and strategies for adoption of more materials production and use under the sustainability concept. At individual level, the behavioral changes towards a more sustainable way of living and consumption are strongly influenced by the knowledge regarding the subject.

The present paper presents an initiative supported by the Erasmus+ project EDU4PlastiCircular - "Education for Plastic in a Circular and Climate Neutral Economy - Preventing Waste Ending Up into the Environment" (Project No: 2023-1-RO01-KA220-HED-000166242), gathering a partnership comprising of Universita degli studi dell'Insubria (Italy), Faculty of Environmental Protection Velenje (Slovenia) Dermol svetovanje, d.o.o. (Slovenia), Universitat Politecnica de Valencia (Spain) and Transilvania University of Brasov (Romania), under the coordination of Polytechnic University of Timisoara (Romania). The three-years project (2023 – 2026) aims to develop and boost the green skills of higher education institutions teachers and students, managers and employees, and green practices and awareness for plastic in circular economy and neutral economy and to contribute to the EU's digital transformation by: (1) Creating innovative training methods and reference process framework based on best practices of education and (2) Releasing open training materials, e-learning platform and upskilling at least 200 learners.

PB16. VIS-ACTIVE PHOTOCATALYTIC THIN FILM BEADS FOR WASTEWATER TREATMENT

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Advanced wastewater treatments, like photocatalysis, can eliminate traces of pollutants (in the ppm range). Photocatalysis uses metal oxide semiconductors to degrade organic pollutants, under VIS or solar radiation (ideally). The best known photocatalyst is TiO_2 which is chemically stable, low-cost and highly efficient. To extend the activation domain of TiO_2 from the UV to the VIS spectral range, the metal oxide can be coupled with carbon derivates, such as gC_3N_4. The composite materials can be used either as (nano)powders (with higher specific surface and thus higher efficiency) or as planar thin films (which are easier to remove from water and to reuse). A novel alternative proposed in this work is the deposition of thin composite sol-gel films on glass beads in order to maintain the high surface area with easy retrieval, regeneration and reuse.

The thin films are obtained in two steps. The first step includes the deposition of a pure TiO_2 layer starting from a sol of titanium isopropoxide, ethanol, acetylacetone, acetic acid and water (20:16:0.89:0.18:2.4 vol) that is ultrasonicated for 90 min. One gram of beads is immersed in 5 mL of sol, under constant stirring (30 min). Drying is done at 110 ^oC for 1 h, followed by annealing at 450 ^oC for 3 h. Similarly, a second, TiO_2-gC_3N_4 layer is deposited from a sol, to which a gC_3N_4 ethanolic dispersion is added in order to obtain a 5% carbon derivate filler in the thin film. All other deposition parameters are maintained from the first deposition.

Photocatalytic tests against methylene blue (MB) and imidacloprid (IMD) with the initial concentration 10 ppm, under UV+VIS (G = 35 W/m²) and UV (G = 5W/m²) radiation showed that all samples were VIS-active and suffer no clogging even after 9 h of testing. Adsorption plays only a small role in the MB degradation (<5% compared to the overall ~70%), whereas it is much more significant in the case of IMD (10% adsorption to 45% overall removal efficiency).

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PB17. CURRENT CHEMISTRY OF NUNTAȘI LAKE AND ITS TEMPORAL CHANGES

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Located approximately 35 km north of Constanța, on the Black Sea coast, Lake Nuntași-Tuzla is part of the Razim-Sinoe lakes complex, integrated into the Danube Delta Biosphere Reserve. The area is rich in archaeological findings, including late Roman settlements, emphasizing the cultural and spiritual value of the region.

The geochemical analyses, carried out on the surface sediment samples collected from the Nuntași Lake, sought to determine the concentrations of $CaCO_3$, TOC, and some trace elements (metals) with genetic or toxic significance and potentially affected by the anthropogenic influences. To evaluate the degree of sediment contamination, samples were collected from the upper layer of sediments to determine metals: Ti, V, Fe, Cr, Mn, Fe, Ni, Cu, Zn, As, Rb, Sr, Zr.

The analyses were carried out by energy dispersive X-ray fluorescence spectroscopy (XRF) and titrimetric methods. $CaCO_3$ concentrations in the selected sediments recorded concentrations between 6-12%. The TOC values indicate the existence of sandy and well-aerated sediments in the studied area. The results obtained for the content of heavy metals reveal significant correlations: $CaCO_3$ is significantly correlated with Cr and Sr, Ti is correlated with Zr and V is correlated with Fe, Ni, Cu, Zn and Zr.

This information is useful for comparative analysis of the hydrochemical characteristics of Nuntași Lake and allow to assess the water quality of the lake as a whole and in its individual areas.

SECTION C: PHYSICAL CHEMISTRY

OC1. POLYMER BLENDS BASED ON POLYIMIDES CONTAINING TRITYL-SUBSTITUTED TRIPHENYLAMINE FOR CO_2 SEPARATION MEMBRANES

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Aromatic polyimides have been studied intensively due to their excellent properties, such us thermo-oxidative stability, chemical resistance, low dielectric constant, low refractive index, which make them useful for advanced technologies [1]. Lately, these polymers have attracted significant interest for use as gas separation membranes with both high permeability and selectivity besides superior physical and mechanical properties. Polyimides containing trifluoromethyl or hexafluoroisopropylidene groups [2, 3] are among the most attractive for this purpose. However, the low gas permeability despite high selectivity limits their practical use. Thus, polymer blending appeared as a viable route towards efficient gas separation membranes. By blending, a new material with distinctive properties is obtained through a simple, reproducible, and low-cost method. Specifically, blending a fluorinated polyimide with a polyimide containing high free volume [4], is expected to provide high performance gas separation membranes. Along these lines, here we report on the synthesis of some polyimides containing bulky trityl-substituted triphenylamine, that were further employed to obtain a series of polyimide-based miscible blends. Besides detailed structural and physico-chemical characterization of the polyimides, the polymer blends were investigated with regard to the component's miscibility, thermal, mechanical and dielectric behavior, with a special concern on their potential for use as materials for gas separation membranes.

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OC2. TRIPHENYLMETHANE BASED-POLYIMIDES: SYNTHESIS AND CHARACTERIZATION

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Polyimides have been widely studied for use in microelectronics, sensors, energy storage, biomedical and aerospace engineering industries due to their combined properties such as high thermal stability, mechanical strength, chemical resistance, dielectric properties, and biocompatibility. For example, polyimides have been successfully used in developing polymeric membranes with intrinsic porosity for sustainable CO_2 capture [1]. Moreover, since polyimides represent an extremely important class of polymers in terms of applications diversity, a very important aspect is the solvation capacity because they often have to be manufactured in form of films, membranes, fibers, foams, composites, adhesives, etc. This aspect can be achieved by introducing 3D groups such as triphenylmethane, triphenylamine, etc., and/or by attaching a bulky unit to the side chain, such as aromatic polycyclic unit or different chromophoric groups as phenoxazine, carbazole, etc. Such structural designs certainly lead to applicable polyimides in various high-performance fields, including the area of gas separation membranes but also in advanced materials technologies due to the excellent combination of thermal attributes (including stability and low flammability), good mechanical strength, chemical resistance, dielectric properties, etc. Therefore, in this study, a new diamine based on triphenylmethane (TPM) was synthesized and used to obtain novel polyimides. Detailed investigations on the chemical structure, photo-optical, thermal and electrochemical behavior were accomplished to survey the structure-properties relationships promoted by the polymer structural variation relevant for applications in advanced technologies.

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OC3. MASS SPECTROMETRIC CONFIRMATIONS REGARDING MECHANISTIC INSIGHTS IN THE DOEBNER REACTION

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The Doebner Reaction is a well-known method for synthesizing carboxyquinolines from aniline derivatives with electron-donating groups. However, aniline derivatives possessing electron-withdrawing groups, like iodine, yield different products, notably 1H-pyrrol-2(5H)-one derivatives. In this study, we aimed to investigate the mechanism behind the formation of new iodo-carboxyquinoline derivatives. Important mechanistic insights were gained through mass spectrometry (ESI-MS, MALDI-MS) and NMR techniques.

By conducting ESI-MS and MALDI-MS analyses on the reaction mixture at distinct time intervals, we obtained compelling evidence confirming the gradual consumption of the starting compounds. Furthermore, the relationship between structure and reactivity was investigated through computational analysis. This comprehensive approach allowed us to elucidate the reaction mechanism and confirm our findings through theoretical studies.

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PC1. STRUCTURAL INVESTIGATIONS OF POLYESTER RESINS WITH ANTHRACENE-PROTECTED MALEIMIDE GROUPS USING MASS SPECTROMETRY AND THERMAL ANALYSES

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Polyester resins based on diglycidyl ether of bisphenol A (DGEBA) and allyl-modified DGEBA, with maleimide groups protected by anthracene, were investigated using mass spectrometry-electrospray ionization (ESI-MS) and various thermal analysis techniques, including conventional, HiRes TGA, and modulated TGA (MTGA). Through ESI-MS analysis we identified species with anthracene-protected maleimide groups, indicating minimal secondary reactions during synthesis for DGEBA-allyl-Anth. Furthermore, the multiple charged ions detected in the ESI-MS spectrum suggest that the molecular structures of the species associated with the sample DGEBA-allyl-Anth can include approximately 5 anthracene-protected maleimide groups. The TGA investigations confirmed the cleavage of the maleimide–anthracene adduct for DGEBA-allyl-Anth. Overall, these findings provide insights into the thermal behavior and chemical transformations of polyester resins containing anthracene-protected maleimide groups.

PC2. THERMOPHYSICAL AND EXCESS PROPERTIES OF BINARY BLENDS OF BIODIESEL WITH DIETHYL ETHER, DIETHYLENE GLYCOL DIMETHYL ETHER AND DIMETHYL CARBONATE AT DIFFERENT TEMPERATURES

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The physicochemical properties of biodiesel blends are significant for designing injection system components and comprehending the interactions inherent in the mixture. In the present study, density, viscosity, surface tension, and refractive indices of binary blends of biodiesel + diethyl ether (DEE), diethylene glycol dimethyl ether (DGM) and dimethyl carbonate (DMC) which are used as biodiesel additives have been measured over the whole range of concentration from 288.15 K to 323.15 K and at atmospheric pressure. The density and kinematic viscosity values of the binary blends, prepared with different mole fractions of DEE, DGM and DMC, were compared with the limits specified by the biodiesel standard (EN14214). Excess molar volumes (V^E), deviations in kinematic viscosity ($\Delta\eta$), surface tension ($\Delta\sigma$), refractive indices (Δn_D) and excess Gibbs energy of activation of the viscous flow (ΔG^{*E}) values were calculated. These deviation values from ideality were adjusted to a Redlich–Kister polynomial equation and the obtained parameters in the equation were reported.

SECTION D: PETROLEUM TECHNOLOGY AND MANAGEMENT

OD1. THIOPHENE BASED HYPERBRANCHED POLYMERS FOR ELECTROCHROMIC AND ENERGY STORAGE APPLICATIONS

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Efficient energy storage is a rapidly growing and critical field that focuses on developing processes and technologies for converting and storing energy. These advancements are essential for effective utilization of renewable energy sources. The glaring disparity between the location and timing of energy production and consumption necessitates the design and development of new, effective energy storage systems. Also, electrochromic materials are currently being extensively studied for applications in smart windows, plastic electronics, solar cells, and energy storage devices. Thiophene-based macromolecular frameworks are commonly utilized in the fabrication of energy storage and electrochromic devices due to their excellent electrical conductivity, low oxidation potential, stability, unique optical properties, thermal stability, and strong environmental compatibility [1, 2].

Along these lines, this work focuses on creating a system that includes both electrochromic and energy storage functions into a material based on hyperbranched-thiophene polymers. We focused on design, synthesis, and optimization of polythiophene structures and establishing reliable relationships between the structure and the desired properties. Emphasis is placed on: (i) the mechanisms causing the reversible color change; (ii) meeting the criteria for energy storage, and (iii) achieving color changes during electrical charge/discharge cycles.

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OD2. EXTRACTION OF CELLULOSE FROM *ULVA LACTUCA* ALGAE AND ITS USE FOR MEMBRANE SYNTHESIS

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Green algae are a sustainable source of biopolymers for the global demand due to their high photosynthetic efficiency. This study describes the extraction of cellulose from plant systems represented by *Ulva lactuca* species. In order to extract various substances, with the help of solvents (liquid media), from algae, these are finely grounded. This is done to achieve the necessary conditions that help reduce the resistance this phase shows in regard to the transport and transfer of the species being extracted. The highest yield of extracted cellulose (20,944%) was obtained for the following factors: S/L=1/20; conc. ethanol=90%, conc. salts=4g/L.

Hydrogel membranes are a unique class of macromolecular networks that contain a large fraction of aqueous solvent within their structure. With the cellulose extracted from algae, we obtained membranes which underwent the process of swelling in liquid media (ethyl alcohol) of different concentrations. The swelling of biocellulose membranes in alcoholic solutions of high concentrations was investigated. It was observed that the process of absorption of the alcoholic solution by the membrane, occurred rapidly in the first part. After stabilization, the membranes continued to absorb at a slower rate until stabilization or saturation concentration was reached.

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PD1. CONJUGATED POLYMERS BASED ON THIOPHENE FOR USE AS ELECTROCHROMIC AND CAPACITIVE MATERIALS

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From their discovery, conjugated polymers have been studied as electrode material for electrochemical sensors and energy storage devices, due to their chemical diversity and excellent attributes, like adjustable conductivity, structural flexibility and easy coating [1]. One of the most important classes of conjugated polymers are polythiophenes, that display relatively stable conductivity and good optical transparency, suitable for use in electrochromic devices [2], but also the ability to store electrical charges, being promising candidates as electrode materials in supercapacitors [3]. Many synthetic strategies to obtain polythiophenes have been described till now, such us electrochemical, chemical oxidative and transition metal-mediated polymerization. Among them, electropolymerization is a simple, practical and inexpensive way to generate desired surface structures of modified electrodes for various applications. These materials can also change their color as a function of an applied potential, a phenomenon known as electrochromism [4]. From our knowledge derivatives based on thiophene have been very little studied as both electrochromic and capacitive materials [5]. Therefore, our work is focused on developing two propylene-dioxythiophene-containing polymers that were electrogenerated directly on conductive surfaces. Their energy storage performance was investigated by cyclic voltammetry and galvanostatic charge-discharge, while their electrochromism was assessed by spectroelectrochemistry and chronoamperometry.

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PD2. NON-CONJUGATED ProDOT-BASED POLYAMIDES FOR ELECTROCHROMIC CAPACITIVE WINDOWS

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The enormous demand for energy due to rapid technological developments pushes mankind to the limits for the exploration of high-performance energy devices. In this regard, electrochemical capacitors play a crucial role in the storage and supply of conserved energy from various sustainable sources. On the other hand, electrochromic materials have been applied in the industry of intelligent windows and electrochromic displays to save energy. By integrating the energy storage and electrochromism functions, the electrochromic capacitive windows (ECW) are of major interest due to their unique energy-saving and energy-recovery characteristics [1]. With the aim to contribute to this appealing research field, our work is focused on the development of novel three aromatic polyamides containing propylenedioxythiophene (ProDOT) units in the main chain as electrode materials. The polymers were obtained by polycondensation reactions between aromatic diamines with variable structure, planarity and flexibility and a ProDOT-based diacid. Besides some insights into the structural and opto-electronic characteristics of the polymers, their behavior as electrochromic and capacitive materials is reported. Also, a prototype capacitive polyamide based-ECW device was built and its overall performance was investigated. This work demonstrates that non-conjugated polymers containing electroactive units are suitable materials for ECW applications.

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PD3. RECYCLING AND VALORIZATION OF COMPONENTS FROM END-OF-LIFE VEHICLES THROUGH ADVANCED AND SUSTAINABLE TECHNOLOGIES

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The recycling and valorizing of materials derived from the dismantling of end-of-life vehicles (ELVs) have emerged as crucial research topics in sustainability and environmental protection. Given the low levels of recycling and valorization of auto components in Romania, feasible research studies are imperative for the entire process of valorizing materials from ELVs. Globally, the current trend involves using multiple plastic waste streams as raw materials in treatment facilities through catalytic depolymerization, transforming waste into alternative energy resources. From the disassembly stage of ELVs conducted between April and June 2023 at a specialized facility, an average of 64 kg of polymeric materials and 28 kg of elastomers (rubber) were recovered from 55 processed vehicles (with a net weight < 3.5 t). Plastics constitute approximately 11.5% (14.8%, according to ADEME, 2017) of the total materials separated from exterior and interior auto components. Variable quantities ranging from 50 to 100 g of rubber obtained from ELV disassembly underwent a thermal treatment in a pilot-scale depolymerization facility operating in batch mode. Results from gas chromatography analyses indicate a rich content of saturated aliphatic hydrocarbons (C_1 – 12.24% v/v; fraction C_2 – C_6) and unsaturated hydrocarbons (C_2 – 17.87% v/v; C_3 – 7.56% v/v) with high energy potential. The calculated average calorific power value of approximately 50 kJ/g for the treated product suggests the effectiveness of the thermal treatment process.

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PD4. PERFORMANCE EVALUATION OF A THERMOELECTRIC COOLING BOX SYSTEM

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Thermoelectric cooling (TEC) technology has proved to be an efficient refrigeration method for various domestic applications, such as a cooler box for food storage [1] or a thermoelectric air conditioning system [2]. The Peltier-based TEC refrigeration modules offer portability, lightweight, and compactness with low maintenance and operations costs, being powered by DC electrical sources like solar photovoltaic (PVs) systems comprising solar panels, a charge controller, storage batteries and a DC–DC converter [3]. The main drawback of the TEC refrigeration system is its low value of the coefficient of performance (COP) and, thus, is not suitable for high cooling capacities. Heat transfer optimization at the cooler hot side and a proper TEC module selection can enhance the COP at values over 0.5, usually registered for a TEC operating under a temperature gradient ΔT of 20°C. We investigated the refrigeration capacity of a thermoelectric–based cooling box system comprising two different TEC modules, TEC1 – 12705 and TEC1-12706, characterized by power supply values of 44.16 W and 54 W, respectively. We used a thermally isolated box made from expanded polystyrene with a cooling capacity of 3.38 l. After ten minutes of testing, the air inside the box was cooled at similar values of about 11ºC for both TEC modules, starting from the initial temperature of 24ºC. Nevertheless, the cooling system comprising TEC1-12705 had a COP value of 0.86 at ΔT= 20°C, which was 19.4 % higher than in the TEC1-12706 based system.

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PD5. ONE-DIMENSIONAL THERMAL MODEL FOR TEMPERATURE EVALUATION INSIDE THE WATER – COOLED PEMFC

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Proton Exchange Membrane Fuel Cell (PEMFC) systems generate a high amount of heat under normal operation conditions, equivalent to about 45 – 60 % of the total energy content of hydrogen [1]. For this reason, a proper cooling technique has to be used for efficient PEMFC thermal management. A liquid cooling system is preferred in several practical applications of high–power PEMFC stacks (over 1 kWe) due to the superior thermal capacity and improved heat transfer properties of liquid coolants (water) compared to air [2]. This study used a one – dimensional heat transfer model to investigate the temperature distribution at various interfaces between the fuel cell components: cooling channel/bipolar plate (BP), BP/gas diffusion layer (GDL), and GDL/catalyst layer (CL). The main geometrical and thermo-electrical parameters of a portable PEMFC stack with a nominal electrical power of 1 kW were considered in this case. We performed here a parametric analysis to evaluate the heat transfer improvement through the BP of the fuel cell by modifying the water heat transfer coefficients at forced convection and the electrical and thermal conductivities of the BP material based on a composite matrix of graphite, resin and in–situ deposited multi-walled carbon nanotubes (MWCNTs) [3].

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PD6. OPTIMISATION OF OIL PRODUCTION FUNCTION TO POROUS ROCKS

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The exploitation of fluid hydrocarbon deposits and the extraction through wells of the crude oil and gas contained in these deposits constitute one of the oil industry's most essential and representative areas. On the one hand, this fact was determined by the increase in demand worldwide and, on the other hand, by a higher economic efficiency of exploitation. By applying classic extraction methods, the recovery factor of crude oil from a field is estimated at approximately 30%. By applying new technologies, the value of the recovery factor can increase up to 50...60%. The technological regime established for each well must ensure exploitation at optimal parameters. For this, it is necessary to know the causes that contribute to the decrease in flows and the most effective measures for their prevention and liquidation, which can be attributed to the choice of bottom or surface equipment and the productive layer. These causes can be determined through rigorous and competent control of the installation operation and the quantitative and qualitative analysis of the results obtained through the various measurements performed at the pumping wells. The extraction of crude oil by pumping is widely used in our country, but the yields of many wells are relatively low, either due to the exhaustion of the strata or the equipment used in the extraction process. The piston pumps used in this method operate at low efficiencies or get blocked in conditions where the percentage of impurities and the gas-oil ratio are high. To eliminate these inconveniences, helical pumps are increasingly used to work at high yields, even in water and gases.

This article aims to optimize the operating regime and reduce the energy and material consumption of some wells on structures B on a group of deposits L, as well as design the technological regime of their operation in different exploitation systems.

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PD7. SEPARATION OF WATER FROM NATURAL GASES

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Multiphase flow can be defined as the simultaneous flow through a defined surface of multiple phases interacting or moving (sliding) independently, one next to the other.

The study of multiphase flow is critical in the energy industry, especially in oil and gas extraction.

The transport of two-phase gas-liquid mixtures through horizontal, vertical, or inclined pipelines is encountered in the crude oil extraction industry, industrial processes, in chemical reactors, the flow of fluids through heat exchangers, and even in cooling/condensing processes.

The biphasic flow (gas-liquid, liquid-solid, gas-solid) causes an appreciable increase in the pressure drop during the processes.

Several calculation methods for pressure gradients (Δp/l) and other elements characteristic of movement are available in the specialized literature. In this study, there are discussed the well-known calculation methods, namely the Lockhart-Martinelli and Brill-Beggs methods.

A method is proposed in this work, which aims to reduce the water content of natural gases and consequently, to reduce the energy consumption in gas transportation system.

Water separation by mechanical methods must be considered because of the transport systems appreciable length and if correctly chosen, these methods can be effective for a long period of time.

Apart from these considerations, the mechanical methods also have the advantage of using the energy of the transported gases to disperse the water in the gas mass, so the gas will be transported along the pipeline with a force sufficient to achieve this transport. The modelling of these forces (advance resistance forces) represents the scientific novelty of this work.

[1]. D. Bârsan, T. Sandu, M. Helstern, T. Chiș, EmergeMAT - 5th International Conference on Emerging Technologies in Materials Engineering, Book of abstracts, p. 20, Bucharest 2022.

PD8. TREATMENT OF HYDROCARBON-POLLUTED WATERS THROUGH OXYGEN AND OZONE NANOBUBBLE TECHNOLOGY

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The system that this paper considers to best respond to the application of treating water polluted with hydrocarbons is the one with solid separation and significant hydrocarbon components, supplemented with ozone and oxygen nanobubbles, combined with devices to increase the reactivity of the components by vortex effect and permanent magnets.

The application presented is washing barges and containers carrying fuel or petroleum products between uses. The resulting water has the necessary and sufficient composition to resume the technological process without being additionally treated or exchanged with fresh water. The installation does not process oil waste; it will be transported to a unit specialized for this operation. The installation is in a closed circuit, starting from clean water, charged with nitrogen nanobubbles - to facilitate the detachment from the barge walls or transport wagon of the attached petroleum products. It is then discharged with the pump to the primary separation basin of solid particles and heavy hydrocarbons. The nanobubble installation, powered by an air compressor, introduces ozone nanobubbles into the water after the first separation, followed by treatment in the second container. The fraction of light hydrocarbons from the water is also separated in this reactor. The light hydrocarbons are collected and discharged into the hydrocarbon container. The resulting hydrocarbon-free water is treated with ozone again in a second reactor, after which it is fed to the high-pressure pump to resume the barge/wagon wall cleaning circuit.

In conclusion, based on these technologies - ozone, oxygen, nanobubbles - it is possible to create water treatment facilities polluted with hydrocarbons, removing the hydrocarbons and recycling them in a separate circuit, but obtaining clean water to resume the technological process, return it to nature, or, following a more complex process, make it potable for agriculture and consumption.

[1]. D.O. Cîrjan, M. Stoicescu, C. Panaitescu, Romanian Journal of Petroleum & Gas Technology IV (LXXV) (2023) 239-250.

PD9. REZERVOIR OPTIMISATION OF OIL PRODUCTION BY IPR CURVES

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A complete oil and gas production system consists of a reservoir, well, production pipeline, separators, pumps, and transport pipelines. The field supplies the well with crude oil or natural gas. The probe provides a path for the produced fluid to flow from the productive formation to the surface and controls the fluid production rate. The mixing pipe directs the produced fluid to the separators. Separators remove gases and water from crude oil. Pumps and compressors transport oil and gas through pipelines to points of sale. *Reservoir production capacity* is defined as the oil or gas production rate achievable from a well in a given period of time under certain conditions of pressure and temperature. A significant factor affecting the production capacity of wells is the bottom pressure. The production capacity of the deposit determines the types of completion and artificial lifting methods to be used.

The reservoir's production capacity depends on the following factors: reservoir pressure, thickness and permeability of the production zone, type and distance of reservoir boundaries, wellbore radius, properties of the fluid in the reservoir, near-wellbore conditions, and relative permeabilities of the reservoir.

Reservoir production capacity can be mathematically modeled based on flow regimes such as transient flow, steady-state flow, and pseudo-steady flow. Mathematical models can describe how a reservoir produces hydrocarbons as a function of variations in pressure and other parameters. The well's flow rate as a function of bottom pressure characterizes the flow through the reservoir, which defines the well's behavior curve (IPR—"Inflow Performance Relationships").

This paper addresses the procedures for establishing IPR curves for various reservoir types and well configurations.

[1]. R.S. Mohammad, D. Iancu, D. Stoianovici, T. Chis, SICHEM 2022, Book of abstracts, p. 20, 2022.

PD10. OPTIMISATION OF GAS STORAGE

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In the coming years, technical, economic, and political factors will determine a rapid increase in the demand for natural gas worldwide. In recent years, the increase has been over 2% per year.

The current functional storage capacity is equivalent to 11% of world consumption, but keeping this percentage means an increase of 85 - 110 billion m^3.

Residential and commercial consumption will reach 25% of total consumption. Population growth and the diversification of energy resources will increase gas demand worldwide.

Although global gas production does not pose problems - being able to cover growing consumption - there are several other problem factors such as production availability, gas transportation from producers to high consumption areas, infrastructure, political and strategic issues, etc. That is why the warehouses will have to be built on the one hand in the producing/exporting countries and the countries located in the transit area. On the other hand, the consuming/importing countries will have to build a strategic reserve to cope with system interruptions and negotiate contractual payment terms better.

On a global level, two trends are foreseen:

1. The construction of small capacity warehouses that are very flexible regarding the reversal of injection extraction processes;

2. Building warehouses with large capacities to ensure strategic reserves for the respective country.

To increase the efficiency of the storage-extraction process, a turboexpander is recommended during the extraction cycle.

It is being analyzed, and it is desired to create a deposit in the area of the Moldova platform (in one of the deposits: Roman, Mărgineni, Tazlăul Mare, or Todirești) with a functional storage capacity of 1-2 billion m^3/year.

[1]. L.I. Tarnu, T. Chis, D. Stoianovici, R.S. Mohammad, International Journal of Education and Information Technologies 17 (2023) 128-133.

PD11. THE EFFECT OF CO_2 ON COLLECTOR ROCKS IN OIL FIELDS

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The extremely low porosity and permeability, substantial heterogeneity, and low energy of depleted crude oil reservoirs result in low recovery of petroleum fluids. CO_2 is the most helpful gas (both for reducing the pollutant footprint and especially for its mobility) and is more accessible to injection. This gas increases the mobility of crude oil, which leads to CO_2 injection being widely used to improve crude oil recovery from depleted deposits and viscous crude oils (CO_2 - EOR - Enhanced Oil Recovery - Increase in Oil Recovery). However, problems related to the low solubility of CO_2, the low pressure at which the fluids are present in the reservoir, and the need for the injected fluid to reach the miscibility state limit the improvement in crude oil recovery. Several methods have been proposed in recent studies. In this study, attention will be paid to the CO_2 injection method as a cosolvent to increase the efficiency of crude oil extraction and CO_2 storage. CO_2 injection mechanisms as a cosolvent result in its dissolution in crude oil in order to reduce the interfacial tension between the petroleum phases and increase the competitive adsorption between the two phases. So far, the following facts have been found by molecular simulation: ether groups can improve the solubility of CO_2 in crude oil, and the interfacial tension between CO_2 and crude oil is effectively reduced by dimethyl ether, methanol, or ethanol added, which can improve the recovery of crude oil. It was also found that the promoting effect of acetone as a cosolvent in extracting heavy hydrocarbons was more substantial than that of alcoholic cosolvents.

It was demonstrated that the solubility of CO_2 in alkanes increases with increasing concentration of ethyl acetate added. Good progress has been made in the research of CO_2 cosolvents for increasing crude oil recovery, but the effect of nanopore isolation of reservoirs has yet to be considered.

[1]. T. Sandu, M. Helstern, D. Bârsan, T. Chiș, EmergeMAT - 5th International Conference on Emerging Technologies in Materials Engineering, Book of abstracts, p. 19, Bucharest 2022.

PD12. EFECTS OF ACID TO OIL ROCKS

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The energy demand will almost double in the next 20 years. Humanity consumes about 19 billion tons of oil equivalent (for a population over 8 billion inhabitants). From now, the population is expected to be in slight decline, however it is predicted that about 32 billion tons of oil equivalent per year will be consumed in 2040. Renewable energy solutions are under development, but as a transition fuel, natural gas will remain an energy support with growing demand. That is why new natural gas reserves are being sought, and attempts are being made to increase production from existing deposits. This paper aims to present a new and faster way to fracture and stimulate the production from unconventional formations (such as shales or clays) from an onshore well. Formation stimulation was performed by making multiple acid fracturing treatments evenly spaced along the horizontal wellbore. The main contribution of this work is the mathematical modelling of acid fracturing processes. Also, it was studied a new recipe for chemical substances with applications in hydra-jet acid processes. The abrasive and acid-soluble mixture is intended to create a new fracturing technique that can be extended to other drilling in carbonate rocks or clays. The use of a one-way coiled tubing operation saves time, money, and effort. The proposed treatment consists in a multi-jet treatment step with a cross-linked gel solution designed to create the fracture, a crack enlargement step based on a gel-hydrochloric acid solution (HCl 15%) and a stage of transporting/ pushing this solution (gelled acid) into the fracture. Subsequently, pumping operations are discontinued, allowing sufficient time for the fracture to develop. Then, a quantity of 15% HCl solution is pumped at a low rate into the fracture to improve the conductivity of the rock (in a technique called *closed fracture acidizing* or *CFA*). Later, this acid will be transported into the rock to be eliminated in chemical reactions so as not to corrosively destroy the metallic walls of the well.

[1]. A.O. Pozo, A. Zeinab, T. Chiș, C.M. Brezeanu, A case study to using acid soluble abrasive materials for hydra jetting gas well, Mining Revue 29 (2023) 80-86.

PD13. CORROSION IN ROMANIAN OIL PLATFORMS - A CASE STUDY

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Offshore structures, both fixed and mobile, are metal or metal-reinforced concrete constructions intended to support oil and gas exploration and production installations under conditions of extreme external demands such as loads as a result of gravity (the own weight of the installations), loads developed by environmental factors (wind, waves, sea currents, marine vegetation), seismic loads or even accidents. Thus, the components of offshore structures can be subjected to permanent stresses of various intensities (horizontal or vertical movements, vibrations), which can rise the mechanical stress. Also, the corrosion of the components plays a vital role in the degradation of the installations. An impressive number of offshore structures are designed to comply with the provisions and international standards in force on the world's seas and oceans. These standards discuss the type of request, the structural analysis of each type of installation, and the required checks. The design of an offshore installation is analyzed to meet all the requirements and robustly cope with both normal exploitation and extreme conditions. Significant design changes during operation lead to a reassessment of structural integrity, which the updated design project must perform. In this case, new structural resistance calculations will be made to ensure that the requirements of the regulations are met.

In the Romanian territorial waters of the Black Sea, several fixed installations were built before 1989 or in the following years, installations that followed the Romanian standards of the time; just a few have considered the international standards in the design phase. Currently, they show signs of degradation due to environmental factors that have acted on them over the time or due to ineffective maintenance. This is why, in this paper, the presentation of their condition and the measures that must be imposed to extend their life are presented.

[1]. D. Iancu, D. Stoianovici, D. Bârsan, T. Chis, SICHEM 2022, Book of Abstracts, p. 122, Bucharest 2022.

PD14. ODORIZATION OF NATURAL GAS - A CASE STUDY

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The work presents the conditions for the odorization of natural gases. Among the substances with a specific smell used in the natural gas distribution industry, compounds with nitrogen, ammonia, amines, amides, nitriles, esters, ethers, natural extracts (aromatic derivatives, sulphur derivatives), etc. are employed.

It should be noted that the organic sulphur compounds are preponderant in this industry. In this category of compounds, thiols and thioethers are considered as best odorizing agents responding to required quality.

In this article, the physical and chemical properties of main odorant are presented. Mercaptans have similar properties to hydrogen sulphide.

Following the considerations listed above, the conditions that must be met by a substance to be a good odorant can be deduced:

- To have as little as possible a chemical reactivity.
- To have a specific, intense, and persistent smell.
- To be combustible, and the combustion products should not have toxic properties.
- To maintain their scent as long as possible.
- To be easy to handle, and its vapors should not spread quickly in the environment, to avoid environmental problems.

The use of an odorant is necessary for the security of gas distribution facilities and especially for preventing damage to homes and injury to users.

Even though odorants are dangerous substances in minimum doses (e.g.: order of 1/300000000 to be detected), they do not affect the end user while providing protection against explosions.

[1]. S. Gal, M. Albulescu, R. Rădulescu, T. Chis, Romanian Journal of Petroleum & Gas Technology IV (LXXV) (2023) 144-158.

PD15. A COMPARATIVE STUDY ON APPLICATION PROPERTIES OF DIESEL FUEL BLENDS WITH DIBUTYL ETHER (DBE)

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Physico-chemical properties of dibutyl ether/diesel fuel blends were empirically tested in this study. In particular, kinematic viscosity (ν), cloud point (CP), pour point (PP), flash point (FP), lubricity, conductivity, cold filter plugging point (CFPP), cetane number and water content were examined. For this research diesel fuel was blended with dibutyl ether (DBE) in volumetric ratios of 0,5% 10%, 15% and 20%. It was found that DBE impacts significantly on the improvement of diesel kinematic viscosity (ν), cloud point, pour point, conductivity, cold filter plugging point (CFPP) and cetane number of tested fuels. It was found that DBE impacts significantly on the improvement of diesel kinematic viscosity, cloud point, pour point, conductivity, cold filter plugging point and cetane number of tested fuels. The role of viscosity in the injection process seems to be the most important than any other parameter, therefore it must be set according to the values mentioned in EN590 standards. According to this standard, the kinematic viscosity value of diesel fuel should be between 2 and 4.5 mm^2/s. As the addition of DBE increased, the kinematic viscosity decreased. This is an expected result since DBE has a lower kinematic viscosity value (0.557 mm^2/s) than diesel (3.0727 mm^2/s). The pour point measurements were performed according to the ASTM D 97 analysis method. The introduction of DBE (diethylene glycol dibutyl ether) resulted in the most significant reduction in the pour point (PP) temperature of the diesel fuel, decreasing it from -6 °C to -12 °C at a concentration of 20 vol%. The addition volume of DBE have a minor effect on CP of the fuel. The maximum CP reduction for 15 vol.% of DBE is obtained as -4°. The best results regarding the CFPP showed the additive 20 vol. % of DBE induced the CFPP reduction to -8 °C. The flash point is indeed the lowest temperature at which a fuel will ignite when exposed to an ignition source. Diesel has flashpoints as 60.5 °C. The addition of 20 vol.% of DBE in diesel reduced to 45° C of the flash point. DBE has a negative effect on flash point. The obtained results show that DBE appears acceptable as a fuel additive for diesel fuel.

PD16. EFFICIENT AND ECOLOGICAL PROCESSES IN OBTAINING SOAPS FROM WASTE COOKING OILS

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In the face of increasing environmental concerns and the imperative to transition towards sustainable manufacturing practices, this study explores innovative approaches to soap production utilizing waste cooking oils as a renewable resource. Waste cooking oils, predominantly derived from household and commercial food preparation activities, represent a significant environmental challenge due to improper disposal methods leading to pollution and ecological harm. This research focuses on the development and optimization of efficient and eco-friendly processes for transforming waste cooking oils into high-quality soaps, thereby addressing both environmental and economic aspects of sustainability.

The study commences with the collection and characterization of various waste cooking oils to determine their suitability for soap production based on key physical and chemical properties. Subsequently, a systematic experimental procedure involving saponification, neutralization, salting-out, and purification is employed to convert the waste cooking oils into soap while minimizing waste and resource utilization. The produced soaps are then subjected to comprehensive quality assessment, encompassing physical, chemical, and performance evaluations to ascertain their suitability for diverse applications.

Furthermore, an economic analysis and environmental impact assessment are conducted to evaluate the feasibility, cost-effectiveness, and ecological benefits of the developed soap production processes compared to conventional methods. The findings of this study demonstrate promising results in terms of yield, quality, and sustainability, highlighting the potential of waste cooking oils as a valuable feedstock for eco-friendly soap manufacturing.

[1]. S.N.K. Azme, N.S.I.M. Yusoff, L.Y. Chin, Y.Mohd, R.D. Hamid, M.N. Jalil, H.M. Zaki, S.H. Saleh, N. Ahmat, M.A.F.A. Manan, N. Yury, N.N.F. Hum, F.A. Latif, Z.M. Zain, Cleaner Waste Systems 4 (2023) 100084.

PD17. UTILIZING WASTE COOKING OIL AS LUBRICATING OIL: A SUSTAINABLE APPROACH TO AUTOMOTIVE MAINTENANCE

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With the escalating global demand for lubricating oils coupled with growing environmental concerns associated with the disposal of waste cooking oil, there is an emerging opportunity to repurpose this abundant waste stream as a sustainable alternative in the lubricant industry. This research delves into the feasibility and performance of utilizing waste cooking oil as a substitute for conventional lubricating oils in automotive applications, aiming to mitigate environmental pollution and contribute to circular economy initiatives.

The study initiates with the collection and characterization of diverse waste cooking oils to ascertain their chemical composition, viscosity, and thermal stability, pivotal factors influencing their suitability for lubricating applications. A systematic experimental methodology encompassing purification, modification, and formulation processes is employed to refine the waste cooking oil into a lubricating oil with desirable physical and chemical properties. Some analytical techniques, including, viscosity measurements, and tribological evaluations, are utilized to assess the quality, performance, and compatibility of the waste cooking oil-derived lubricant with automotive engines and machinery.

The research findings reveal promising outcomes, demonstrating that waste cooking oil can be effectively transformed into a high-performance lubricating oil that meets industry standards and regulatory requirements while offering environmental benefits, cost savings, and potential market opportunities.

This study contributes to the advancement of green chemistry, sustainable materials, and automotive engineering by presenting an innovative and eco-friendly approach to lubricant production, utilizing waste cooking oil as a renewable and sustainable resource, and fostering sustainable practices in the automotive and lubricant industries.

[1]. J.R. Joshi, K.K. Bhanderi, J.V. Patel, Journal of the Indian Chemical Society 100 (2023) 100820.

PD18. MODELING POLYMER MOVEMENT IN RESERVOIR ROCKS

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The importance of fluid hydrocarbons, both from the point of view of the energy source and as a raw material for the chemical and petrochemical industry, is attributed to reservoir engineering in terms of increasing the recovery factor of crude oil from the reservoir. Primary, secondary, and tertiary exploitation methods to achieve this goal require appropriate tools to prevent the behavior of the deposit under the specific conditions of the respective recovery mechanism.

The analytical use of the equations of motion to predict the behavior of a hydrocarbon deposit in the exploitation process is limited to a small number of cases that can be solved analytically, but also to the reduction of the quality of the results by the simplifying assumptions on which the analytical solutions are based. Using methods to solve the fundamental equations of fluid movement in hydrocarbon deposits, an essential step towards the knowledge of the phenomena associated with exploiting these deposits was achieved.

The large volume of calculations involved in the numerical solution of the partial differential equations of motion makes numerical modeling viable only under very fast automatic calculation means.

In the modeling, a series of peculiarities can be taken into account, such as the inhomogeneity and anisotropy of the reservoir rock, the variation of the thickness of the productive layer, the interphase transfer of mass and heat, the non-Newtonian behavior of some fluids in porous media, the variation of the properties of fluids and rock with pressure and temperature and so on. In this article, We will solve the problems that arise when simulating the movement of polymers in the context of the displacement of crude oil from oil fields.

[1]. M. Helstern, T. Sandu, D. Bârsan, T. Chiș, SICHEM 2022, Book of abstracts, p. 135, Bucharest 2022.

SECTION E: FOOD CHEMISTRY AND ENGINEERING

OE1. NMR METABOLOMICS OF TOMATOES DEGRADATION

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Tomato (*Solanum lycopersicum*) is one of the most produced vegetables in the world, with 189 million tons in 2021 [1]. The industrial processing of tomatoes generates a large amount of waste on which metabolomic studies could be done in order to characterizing it and monitor its evolution in time. NMR spectroscopy has proven to be one of the most versatile techniques for characterization of primary metabolites in *ex vivo* matrices of vegetal fluids [2].

To date there are no studies regarding the dynamic metabolomic characterization of tomatoes' degradation in various conditions. In the present study we followed over a period of 366 days the metabolism of tomatoes in various simulated conditions. The reproducibility of NMR instruments used for metabolomic studies was also assessed [3].

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PE1. NUTRITIONAL COMPOSITION AND LIPID QUALITY OF BLACK SEA *CHAMELEA GALLINA*

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The white sand clam, *Chamelea gallina*, is a valuable source of biologically active substances. Despite of its nutritional and economic potential, the nutritional composition of *Chamelea gallina* from the Black Sea has been poorly studied. The present study aims to determine the chemical composition of the white sand clam *Chamelea gallina* sampled from the Bulgarian Black Sea coast. Crude proteins, carbohydrates and total lipids were determined by standard procedures. Macronutrients (K, Ca, Mg, Na) were determined by ICP-OES. Fatty acid composition was analyzed by GC/MS. Analyzed samples were characterized by high protein and low lipid content. The total carbohydrates ranged between 0.7-1.6 g/100g ww and the energy value between 99.3 and 101.72 kcal/100 g. The concentrations of the analyzed macroelements ranged between 1527.33 and 2171.43 mg/kg ww for K; 749.50 and 1759.14 mg/kg ww for Ca; 452.95 and 958.52 mg/kg ww for Mg; 1988.43 and 3804.41 mg/kg ww for Na. Lipid classes present in the shellfish oil include neutral, polar lipids, sterols, and sterol esters. Significant differences in the fatty acid distribution were observed between the lipid fractions. The high lipid quality of bivalve mollusks is demonstrated by the predominance of PUFA group in the total lipid fraction. *Chamelea gallina* could be considered as a sustainable and alternative source of n-3 PUFA (33.7-41.9% of total FA). The present study reveals new data on the chemical composition of *C. gallina* from the Bulgarian Black Sea coast. The results show that *C. gallina* could be a very good protein source with high nutritional profile while low in lipid, carbohydrate and calorie content.

PE2. THE MICROGREEN PLANTS - A GOOD ALTERNATIVE FOR HEALTHY HUMAN DIET

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Microgreens are a large group of plant species (over 60 varieties), including young specimens of popular grains, legumes, flowers, and herbs. Their nutritional quality and affordability explain the high and constantly growing interest in them in the last decades. Various statistical agencies reported increasing levels of cultivation and consumption of this types of plants, linking it to the problems of the Covid-19 pandemic. They also predict sustainable growth trends in this interest over the next 5 - 10 years.

Microgreen plants are increasingly being established as functional foods, which cause great scientific and industrial interest in them. They are characterized by great species diversity, taste qualities, high content of a variety of biologically active substances. On the other hand, in their cultivation, serious advantages are their short growth period and minimal cultivation needs, which does not include the use of pesticides. Of particular importance is the possibility of their production not only in an industrial, but also in a domestic environment.

Past pandemic conditions increased the interest of the Bulgarian population in functional foods, especially those that can be grown in domestic conditions. Therefore, the aim of the current literature review was to systematize and popularize information about the benefits of microgreen plants, available on the Bulgarian market, such as micro peas, micro kale, micro radish, micro sunflower, etc.

PE3. COATING FORMULATIONS BASED ON IMINE CHITOSAN DERIVATIVES USED IN FOOD PACKAGING

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In recent decades, the replacement of petroleum-based food packaging by cellulose-based one has become an opportunity of great interest both in the scientific world and in industry due to the problems of environmental protection and optimal storage of food products [1]. Although cellulose-based materials are biodegradable, recyclable and low cost, the hydrophilic nature and porous structure of the paper limits its applicability as food packaging [2]. Therefore, coating paper with certain additives can improve its mechanical and barrier properties, making it functional as food packaging. Among the biopolymers used as coating agents, chitosan is a great candidate due to its bioactivity and ability to improve the mechanical and barrier properties of paper [3]. In this context, the aim of this study was finding a route of improving the paper properties by coating it with chitosan or a chitosan derivative. In this view, chitosan was chemically modified by a condensation reaction with citral, a bioactive and hydrophobic aldehyde, resulting in citryl-imine chitosan. Further, it was casted on the Kraft paper and the properties required for food packaging were investigated by comparison with the pristine chitosan control. Thus, the morphological, mechanical and barrier properties of the coated paper were measured and comparative discussed. It was found that the chitosan-citryl imine coated paper showed both tensile strength, tear and bending strength as well as barrier properties (water absorbency, surface wettability and gas permeability) better than the chitosan coated paper and clearly superior to the pristine paper. As a result, chitosan and chitosan citryl-imine significantly increased the hydrophobicity of the paper, suggesting its utility in the development of eco-packaging.

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PE4. HEAVY METALS LEVELS IN COW'S, GOAT'S AND SHEEP'S FRESH RAW MILK, CURD, AND WHEY FROM DIFFERENT AREAS OF DOBROGEA, ROMANIA

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Heavy metals are often found in the environment, so, the existence of heavy metals in raw milk and its products could be attributed to contaminated drinking water served to dairy animals and/or contaminated feed that absorbed heavy metals from soil that was irrigated with industrial wastewaters. This study was carried out to determine concentrations of cadmium, lead, copper, chromium, cobalt, nickel and manganese in cow's, goat's and sheep's fresh raw milk, curd and whey samples collected from farms in different areas in Dobrogea, Romania. Heavy metals levels were assessed using graphite furnace atomic absorption spectrometry (GF-AAS). Large differences were found between the measured concentrations of studied heavy metals (lower than the quantification limit to maximum concentration). The maximum concentration of Cd, Pb, Cu, Cr, Co, Ni, Mn was 1.92, 37.07, 91.72, 67.90, 49.15, 20.35 1.19 ppm, respectively. In general, higher concentrations were detected in cow's curd samples. Evaporation and concentration of milk in the cheese making process are known to generally increase the concentration of contaminants in dairy products. In addition, heavy metals including lead, cadmium, chromium, and copper have been reported to be preferentially bound to milk caseins and during the coagulation step of cheese processing, are transferred into the curd.

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PE5. PLUM DISTILLED BEVERGAGES QUALITY ASSESSMENT

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This study was performed to investigate the quality characteristics of distilled beverages made from plum fruits. The samples were provided from private manufactures (plum brandy, mix fruits – plum, apple - distilled beverage and plum alcohol) and from supermarket (plum brandy). The total and volatile acidity and alcoholic concentration were determined by refractometric method and, with an oenological system GlassChem. To demonstrate that there are no significant differences between the results obtained by these methods, the t-test was applied and was obtained a t value of 0.19. When comparing the t value obtained with the tabulated t value ($t = 2.78$ for 4 degrees of freedom) it was observed that the calculated $t <$ the tabulated t, the result being statistically insignificant. At the same time $p > 0.05$ which shows that the differences are not significant. The volatile acidity showed a large difference of 1.62–5.46 (acetic acid in grams per liter).

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PE6. TOTAL PHENOLIC CONTENT OF RAW AND COOKED VEGETABLES

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Total phenolic content (TPC) of some raw and cooked vegetables extracts (red and yellow pepper, zucchini, and tomatoes) was studied by a modified Folin-Ciocalteu method. The objective of this work was to validate this method by studding validation parameters such as linearity, precision (in terms of repeatability and intermediate precision), limit of detection (LOD) and limit of quantification (LOQ). A linear calibration for the analytical method over the calibration ranges tested (2 to 12 mg GAE/L) was obtained with $R^2 = 0.9922$. LOD was found to be 0.627 mg/L and LOQ 2.090 mg/L. For both raw and cooked vegetable samples, the time evolution of TPC was followed. TPC ranged from 3.4 to 19.0 mg GAE/100 g product in raw vegetables. The researchers showed that cooking style affected total phenolic content of samples depending very much on the processing time and the size of the vegetables. In this study grilling increased TPC in all studied vegetables (up to 21.8 mg GAE/100 g product).

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SECTION F: MEDICINAL AND PHARMACEUTICAL CHEMISTRY

OF1. ACTIVE COMPOUNDS IN GLYCERIN HYDROALCOHOLIC EXTRACTS WITH POTENTIAL ANTI-INFLAMMATORY EFFECT

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Gemmotherapy, also known as "tree bud medicine", is a branch of phytotherapy that utilizes the medicinal properties of the buds and young shoots of trees and shrubs. This therapeutic approach is based on the belief that these embryonic tissues contain a high concentration of active compounds and vital energy, making them potent sources of natural healing.

Gemmotherapy involves the extraction of these young plant tissues, typically buds, shoots, and rootlets, in a glycerin and alcohol solution. The resulting macerate is then used for therapeutic purposes. The active ingredients present in these embryonic tissues are believed to be more concentrated and bioavailable compared to those found in mature parts of the plant. In this study, gemmotherapy regimens were performed on a group of human subjects aged between 20 and 80 years and we determined the active compounds from gemmoderivates. The gemmotherapy schemes were made with glycerinohydroalcoholic extracts from buds of *Ribes nigrum*, *Rubus fructicosus*, *Rubus idaeus*.

The results obtained after periods of 3 months, 6 months and 12 months have demonstrated the effectiveness and anti-inflammatory effect of these products. The mentioned objectives support the improvement of the health of the body, ensure the intake of bioactive substances necessary for the physiological functions of the hall system.

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OF2. PLANT EXTRACTS RICH IN NATURAL POLYPHENOLS AND FLAVONOIDS WITH LIVER-PROTECTIVE EFFECTS

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Medicinal plants contain bioactive compounds with important pharmacological properties that have been studied for their potential benefits in liver health. Some of these bioactivities include: antioxidant capacity, helping to neutralize harmful free radicals in the body, which can damage cells, including liver cells. Cholestasis is a condition where bile flow from the liver is impaired. Anticholestatic agents help promote bile flow, which is important for the normal liver function. Fibrosis is the formation of excess fibrous connective tissue in the liver, often as a response to injury or inflammation. Antifibrotic agents may help prevent or reduce this fibrosis.

In this work, we study the phytochemical composition, antioxidant activity, and biological properties of *Silybum marianum* and *Cynara scolymus* extracts. We developed dietary supplements as capsules and tablets, that have been clinically tested on a group of human subjects aged between 20 and 80 years; the active compounds from dietary supplements were quantitatively and qualitatively determined and their intake effects were observed and evaluated in large context. The results obtained after periods of 3 months; 6 months and 12 months have demonstrated the effectiveness of these products [1, 2].

The conclusion of the study supports the improvement of the health of the body, by ensuring the intake of bioactive substances necessary for the physiological functions of the liver cells.

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OF3. UNLOCKING THE ANTIMICROBIAL POTENTIAL OF SMALL NITROGEN MOLECULES

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The emergence of antimicrobial resistance poses a significant threat to global health, highlighting the urgent need for novel antimicrobial agents. Small N-containing molecules have garnered attention due to their potential antimicrobial properties. Among various synthetic routes, the Doebner reaction offers a promising approach to synthesize these compounds efficiently [1]. The Doebner reaction, known for its versatility in functionalizing aromatic compounds, enables the incorporation of nitrogen functionalities into the molecular scaffold, thus enhancing antimicrobial properties.

In this study, through careful optimization of reaction conditions, we synthesized a library of diverse nitrogen-containing molecules and investigate their antimicrobial activities revealing potent activity against a panel of clinically relevant bacterial and fungal pathogens.

Acknowledgements: *The support provided by the ICUB Fellowship for Young Researchers (Contract no. 13461/14.12.2023) is acknowledge.*

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OF4. AN EXPERIMENTAL STUDY ON CHITOSAN-BASED HYDROGELS BIODEGRADATION FOR WOUND HEALING

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The skin is the largest organ that protects and thermoregulates the human body [1] therefore, the treatment of skin wounds is of outmost importance for health care system, in continuous searching of effective dressings. Amongst the materials used for this purpose, chitosan-based hydrogels are highly recommended, due to their properties such as non-toxic effect, biodegradability, biocompatibility, and improved ability to re-epithelize and accelerate wound closure [2]. A major disadvantage of commercial wound dressings which should be overcome is their adherence to wounds. In this regard chitosan-based hydrogels are great candidates, that can be adsorbed into the skin during the re-epithelization process thus avoiding traumatic debridement [3]. Although many studies have been carried out on chitosan-based materials, less attention was paid to the pH' influence on their degradation, and this is a very important aspect, taking into consideration that the pH exudate of wounds is varying in a broad domain (9.5 – 5.5) over the healing process. In this light, the aim of this study was to investigate the biodegradation rate of a chitosan-based hydrogel as a function of exudate pH. To achieve this objective, a potential wound healing hydrogel based on chitosan and an antifungal aldehyde was synthesized through an acid condensation reaction. The hydrogel was characterized by FTIR and ^{1}H-NMR spectroscopy and polarized light microscopy and X-ray diffraction, which confirmed the crosslinking mechanism. The hydrogel had good cytocompatibility to NHDF cells and antimicrobial activity against relevant pathogens. In media mimicking the wound exudate, the hydrogel underwent progressive biodegradation modulated by pH, reaching complete degradation in media corresponding to normal dermis, pointing for bioabsorbable wound dressings.

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OF5. NMR LIPIDOMICS

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Following the proven success of genomics and evidence based promises of proteomics, other omics areas are nowadays hot fields of research with high potential of generating future qualitative leaps in life sciences. Transcriptomics, metabolomics, phenomics, or lipidomics are such fields where the scientific research, supported by the high number of publications and high level of funding worldwide, is advancing very fast and which are expected to generate the next major revolution in scientific knowledge.

We apply NMR spectroscopy in metabolomics [1-5] and lipidomics [6-8] for studying complex organisms such as plants [4, 6], animals [5] and humans [1-3, 7, 8] with the purpose of advancing scientific knowledge in food sciences [4, 6], environment [8] and medicine [1-3, 7].

We present some NMR lipidomics results in medical diagnosis, environmental sciences and biomedical research.

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PF1. LIPOSOMES LOADED WITH KAEMPFEROL AS SENOMORPHIC FOR TARGETTING SENESCENT CELLS - OBTAINING AND CHARACTERISATION

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Cellular senescence is a hallmark of ageing and is implicated in various age-related pathologies, including cancer, neurodegenerative diseases, and metabolic disorders. Targeted clearance of senescent cells has emerged as a promising therapeutic strategy to mitigate age-related decline and improve healthspan [1, 2]. Kaempferol, a natural flavonoid abundant in various fruits and vegetables, possesses potent senomorphic properties, capable of modulating key signaling pathways involved in senescence regulation [3]. In this study, we report the preparation and characterization of liposomes encapsulating kaempferol to enhance its stability, bioavailability, and targeted delivery to senescent cells. The liposomes loaded with kaempferol were prepared using thin-film hydration followed by sonication method. The physico-chemical properties of the liposomes with kaempferol, including size and polydispersity index and entrapment efficiency, were evaluated using dynamic light scattering and UV-VIS spectrophotometry. Liposomes loaded with kaempferol exhibited a nano-size and narrow polydispersity index, and good entrapment efficiency (81.54%). Additional in vitro research is necessary to assess the efficacy of kaempferol-loaded liposomes in targeting senescent cells.

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PF2. IR AND UV-VIS SPECTROSCOPIC CHARACTERIZATION OF NOVEL BEXAROTENE ESTERS

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The present study involved the characterization of novel Bexarotene esters thorough the determination of melting points and IR and UV-Vis spectroscopic analysis.

Melting point analysis revealed characteristic temperature ranges for Bexarotene and some of its esters, suggesting successful synthesis but with possible residual unreacted components. The IR spectroscopy provided structural insights, indicating the appearance of characteristic bands associated with the esterification process. Despite similarities in spectra among the esters and Bexarotene, distinct differences were observed, particularly in the region indicative of ester functional groups.

UV-Vis spectroscopy revealed absorption maxima for Bexarotene and its esters in methanol solvent. While the UV-Vis method demonstrated reliability for quantification, it lacks the specificity needed for qualitative differentiation of Bexarotene and its esters due to their structural similarity. Validation of the UV-Vis method demonstrated good linearity, precision, accuracy, and sensitivity, making it suitable for routine quantification of Bexarotene.

Overall, the combination of IR and UV-Vis spectroscopy proved effective in characterizing the novel Bexarotene esters, providing valuable insights into their structural properties and paving the way for further pharmaceutical applications.

PF3. *IN SILICO* PREDICTION OF PHYSICOCHEMICAL PROPERTIES AND DRUG-LIKENESS OF 5-MONO SUBSTITUTED ISATINES

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Isatine holds promise in medicinal chemistry for its potential pharmacological activities, including antimicrobial effects. Given the urgency of combating antimicrobial resistance, exploring the antimicrobial potential of isatine and its derivatives is imperative.

An *in silico* investigation was conducted to predict the physicochemical properties and drug-likeness of 5-mono substituted isatines, utilizing the SwissADME platform. Five isatine derivatives were considered, each substituted with distinct amine moieties: aniline, 4-aminomorpholine, 2-aminopyridine, 3-aminopyridine, and 4-aminopyridine. The physicochemical properties, including molecular weight, lipophilicity, water solubility, and molar refractivity, were determined for each derivative. Additionally, parameters such as the number of heavy atoms, rotatable bonds, hydrogen bond acceptors, and donors were assessed.

The drug-likeness of the substituted isatines was assessed based on several established rules, including Lipinski's rule of five, Ghose filter, Veber rules, Egan's bioavailability score, and Muegge's filter. These analyses aimed to provide insights into the compounds' potential as drug candidates by evaluating their adherence to key criteria associated with oral bioavailability, pharmacokinetics, and drug safety.

Our results reveal that all examined 5-mono substituted isatine derivatives exhibit favorable physicochemical properties and drug-like properties, with no violations of Lipinski's rule of five or other established filters. These findings suggest the potential suitability of these derivatives for further drug development endeavors. By elucidating the structure-property relationships of isatine derivatives, this study contributes valuable insights to the rational design of novel pharmacologically active compounds.

PF4. SYNTHESIS AND REACTION MONITORING OF NOVEL BEXAROTENE ESTERS

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This study presents a novel synthesis methodology for the production of esters derived from Bexarotene, a retinoid X receptor agonist with potential therapeutic applications. The synthesis involves the reaction of Bexarotene with oxalyl chloride in the presence of various primary alcohols to yield the corresponding esters. Four different primary alcohols, methanol, ethanol, 1-propanol, and 1-butanol were utilized under specific reaction conditions. The synthesis process was monitored by observing the complete dissolution of Bexarotene, addition of oxalyl chloride, and subsequent precipitation of the ester product. Different drying conditions were employed based on the alcohol used for synthesis. The results indicate that the reaction proceeds smoothly to yield the desired esters, with some variations observed in reaction kinetics and precipitate formation depending on the alcohol employed. Notably, the use of thionyl chloride as an alternative reagent was found to be unsuitable due to the formation of numerous by-products, complicating the purification process. The practical, theoretical, and percentage yields of the synthesized Bexarotene esters were determined.

The reaction progress was monitored using thin-layer chromatography (TLC) with different mobile phase compositions. Through meticulous experimentation, a 1:1 ratio of hexane to ethyl acetate was identified as the optimal mobile phase for effective separation and identification of the ester products.

This study provides valuable insights into the synthesis of Bexarotene esters, laying the groundwork for future investigations into their potential pharmacological applications and metabolic pathways.

PF5. *IN SILICO* PREDICTION OF PHYSICOCHEMICAL PROPERTIES AND DRUG-LIKENESS OF OMEGA-3 FATTY ACIDS

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Omega-3 fatty acids, including alpha-linolenic acid (ALA), eicosapentaenoic acid (EPA), and docosahexaenoic acid (DHA), are recognized for their crucial roles in human health, particularly cardiovascular and cognitive function. In this study, we employed computational methodologies, leveraging the SwissADME platform, to predict the physicochemical properties and drug-likeness of these essential fatty acids. For ALA, computational analysis indicated a molecular weight of 278.43 g/mol, characterized by moderate lipophilicity (consensus Log Po/w 5.09) and moderately soluble water solubility. EPA exhibited a molecular weight of 306.48 g/mol, along with higher lipophilicity (consensus Log Po/w 5.96) and moderate water solubility. In contrast, DHA, with a molecular weight of 328.49 g/mol, displayed similar lipophilicity to EPA (consensus Log Po/w 5.72) but higher water solubility. Comparison with literature data revealed general alignment in physicochemical properties, such as water solubility and lipophilicity. Furthermore, assessment of drug-likeness according to Lipinski's rule demonstrated compliance for all three fatty acids, albeit with variations in other criteria such as Ghose, Veber, Egan, and Muegge rules. These findings underscore the reliability and applicability of computational approaches in elucidating the physicochemical properties and drug-likeness of omega-3 fatty acids, offering valuable insights for pharmaceutical research and therapeutic applications.

PF6. DRUG-LIKE PROPERTY PREDICTION FOR BIDENTATE LIGANDS BINDING Fe-S CLUSTER PROTEINS

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Fe-S clusters participate in various essential biological processes for the cellular function, such as cellular respiration, nitrogen fixation, sulfur donation, electron transfer, sensing, catalysis, cofactor biosynthesis and others [1]; thus, Fe-S clusters can be used in the development of new therapeutic strategies in numerous human diseases such as type II diabetes, cancer, tuberculosis, malaria and other infections. To identify their opportune application, studies on their structure and role involving different S and/or N ligands, are necessary. In this work, quantum computed investigations on several mono- and bi-dentate ligands reported in the literature data since 2010, as non-hydrogenase [Fe_2S_2] synthetic small molecules [1], are conducted using hybrid algorithm based on Density Functional Theory (DFT), B3LYP [2] with 6-311 G (d,p) basis set by means of Spartan'24 Wavefunction Inc. Irvine CA software [3]. Property prediction was achieved on the minimized structures using Merck molecular force field (MMFF) [5]. Drug-like properties and quantum chemical reactivity parameters were assessed. Based on calculated molecular properties and structural descriptors, the hydrophilic-lipophilic character of the investigated ligands was discussed; their redox active potential was evaluated to further correlate Fe-S clusters applications based on the structure–function relationship and on the nature of their ligands.

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PF7. BIOAVAILABILITY OF SOME NATURALLY OCCURRING ANTHRAQUINONES: A COMPUTATIONAL APPROACH

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Natural anthraquinones derivatives are secondary metabolites structurally related to 9,10-dioxoanthracene and their glycosides. As valuable phytochemicals, these structures received increasing interest of researchers do to their potential as nutraceuticals with therapeutic potency, exhibiting important benefits for human health. In this study, we focus on emodin (1,3,8-trihydroxy-6-methylanthraquinone), an anthraquinone aglycone, commonly found in *Fabaceae*, *Polygonaceae* and *Rhamnaceae* families [1]. It has therapeutic effects in cancer, diabetes, neurodegenerative diseases or chronic inflammatory diseases [2]. To asses its bioavailability, a quantum computed study is conducted using hybrid algorithm based on Density Functional Theory (DFT), ωB97X-D algorithm [3] and 6-31G(d,p) basis set with Spartan'24 Wavefunction Inc. Irvine CA software [4]. Based on calculated molecular properties and structural descriptors, drug-like properties and hydrophilic-lipophilic character of emodin and related anthraquinones were discussed; results could further be applied to find the best therapeutic applications based on the structure–function relationships.

Acknowledgments: *This work was carried out through the "Nucleu" Program, Grant number 1N/2023, PN 23-28 "BioChemLife", within the National Plan for Research and Development and Innovation 2022-2027, carried out with the support of MCID, project no. PN 23-28 04 01.*

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PF8. SYNTHESIS, STRUCTURE AND ANTIMICROBIAL PROPERTIES OF NEW PYRROL 2(5H)-ONE HYBRIDS WITH TRIFLUOROMETHYL MOIETIS

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On October 2020, the WHO declared antimicrobial resistance is one of the top 10 global public health threats facing humanity. In this context, the creation of new classes of antibacterial drugs, with lower toxicity, greater efficacy and lower production costs will be of significant importance for medical industry [1].

One crucial component in the structure of many current antimicrobial drugs are heterocyclic rings. Thus, N-heterocyclic rings are used to enhance pharmacological and pharmacokinetic properties of drugs and to lower toxicity.

The goal of the current study was to synthesize novel bioactive hybrid molecules with pyrrol-2-one as a core and two active binding groups on its sides.

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PF9. OPEN EDUCATIONAL RESOURCES FOR ENVIRONMENTAL AWARENESS OF CITIZENS FROM RURAL COMMUNITIES

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In order to contribute to the environmental challenges, and to the enhancement of environmental awareness and education, Romanian and Icelandic High Education Institutions (HEI), have collaborated in a cooperation project, with support from EEA Financial Mechanism program (2014-2021), in the area of high education.

The "Environmental Education – OERs for Rural Citizens" (EnvEdu – OERs) project was implemented during 2000-2003, with the following partnership: Transilvania University of Brasov, Romania (as project promotor), and Reykjavik University, Iceland, Bucharest University of Economic Studies, Romania and "Gheorghe Asachi" Technical University of Iasi, Romania (as partners).

EnvEdu-OERs project aimed to enhance the quality and relevance of education and training, by developing and delivering new Open Educational Resources (OERs), targeting rural citizens' life-long learning, focusing on environmental awareness, on sustainable rural community development.

The partners produced six teaching modules (TM), developed as OERs video lessons, text-based learning resources, evaluation tests:

- TM1 Sustainable communities and social communication
- TM2 Environmental Quality
- TM3 Environmental Management, Impact and Risk Assessment
- TM4 Waste Management in Rural Communities
- TM5 Water Resources and Water Balance for Sustainable Community
- TM6 Environmental Projects Management

The teaching modules, OERs, are available on the project website (https://envedu.unitbv.ro/en_US/teaching-modules/) as well as on the e-learning platform (https://envedu.unitbv.ro/en_US/envedu-oers-platform/), both in English and Romanian languages.

PF10. NEW PSYCHOACTIVE SUBSTANCE USE: PERCEPTION BY STUDENTS AND TEACHERS

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New Psychoactive Substances (NPS) represent a large and increasing group of chemical compounds characterized by pharmacological and toxicological properties particularly dangerous for the health of consumers. They include stimulants, synthetic substances intended to mimic the effects of controlled drugs and are sold as legal replacements for them.

Aiming to promote student's strengths, their reflexive capacity, and key competencies to tackle the abuse of the above-mentioned substances, the project "Innovative teaching and learning paths for the prevention of new drugs abuse – INES", (2021-1-IT02-KA220-SCH-000032570 - Cooperation Partnership in School Education) was granted with financial support from the Erasmus+ program. The project is developed under the coordination of Bologna University (Italy) and gathers European partners: Porto University (Portugal), Transilvania University of Brasov (Romania), Technical and Economic Institute "G. Salvemini" (Italy), "Mircea Cristea" Technical College (Romania), Secondary School João Gonçalves Zarco (Portugal) and Productions Associees (Belgium).

In this context, a survey was developed to find teachers' and students' opinion regarding the complex and challenging subject of NPS and how it is currently approached in the educational environment. This paper presents the main results of this survey. The topic of NPS is approached in the schools mainly in episodic dedicated activities, or in regular curriculum activities. The didactic approach is more passive (presentations, or video presentation), but respondents (both students and teachers) declared the need of more interactive methods, mainly based on testimonies, case studies, by using video presentations, or video games, etc.

The students and teachers are willing to participate in activities and teaching materials development, but teachers have a sort of caution in expressing their approval, most probably due to the lack of information regarding the subject.

PF11. TAYLOR DISPERSION ANALYSIS: A NOVEL TOOL FOR MONITORING THE AGGREGATION OF β-AMYLOID PEPTIDES

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Alzheimer Disease (AD) represents one of the major public health challenges of the 21st century and its development is centered around the amyloid hypothesis which states that extracellular formation of amyloid plaques and the intracellular accumulation of neurofibrillary Tau tangles (NFTs) are caused by the aggregation of β-amyloid (Aβ) peptides [1, 2]. Several biophysical techniques have been employed for studying the aggregation process of Aβ peptides such as thioflavin T (ThT) assay, dynamic light scattering (DLS), electron microscopy (EM) and atomic force microscopy (AFM). Despite the useful information these methods provide, not all of them are suitable for monitoring the early stages of the process. In this work, we assessed the contribution of Taylor dispersion analysis (TDA) for monitoring the Aβ peptide aggregation mechanism. TDA is a modern technique that can size and quantify soluble species ranging from 0.1 nm to a few hundred nm [3, 4]. We found that TDA revealed that the aggregation process of Aβ(1-40) and Aβ(1-42) isoforms occurs through distinct pathways. We further investigated the co-aggregation of Aβ(1-40):Aβ(1-42) mixture by TDA, highlighting the influence of the peptide ratios on the kinetics and the formation of potentially toxic oligomeric species.

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NOMARES Workshop

ON1. DENSITY FUNCTIONAL THEORY-BASED ELECTROCHEMICAL MODELS FOR TETRAHYDROACRIDINES

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In this research, electrochemical and quantum computed investigations based on Density Functional Theory (DFT) were conducted in order to highlight the correlation between redox potentials and predicted quantum reactivity parameters derived from energetical levels of frontier molecular orbitals. Previous works confirmed the possibility to assess electrochemical properties with good accuracy by quantum mechanical calculations using hybrid density functionals [1, 2]. In the same manner, we used B3LYP/DFT/6-311 (d,p) method [3] to predict quantum chemical reactivity parameters for tetrahydroacridines derivatives and to correlate the calculated energies of HOMO and LUMO orbitals to oxidation, and reduction potentials, respectively. Electrochemical study was performed by cyclic voltammetry, differential pulse voltammetry and rotating disk electrode voltammetry in acetonitrile/ dimethylformamide in presence of tetrabutylammonium perchlorate for different concentrations of each target, at different scan rates and electrode rotation rates. Combination of electrochemical analysis and DFT simulations allowed investigating systematically the effect of different substitution on the thetrahydroachridine skeleton, that affect the electrochemical behavior.

[1]. A.A. Vasile (Corbei), E.M. Ungureanu, G. Stanciu, M. Cristea, A. Stefaniu, Symmetry 13 (2021) 1462.
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PN1. STUDY OF SENSITIVE ELECTRODES BASED ON COMPLEXING AZULENE POLYMER FILMS

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Electrochemical sensors can detect the excess of toxic heavy metals, like lead and cadmium in the liquid medium. Sensitive electrodes based on complexing azulene polymer films were made by electrochemical deposition on glassy carbon electrodes. The chemically modified electrodes (CMEs) were prepared on support of glassy carbon disk, covered by azulene complexing polymer films, 4-(azulen-1-yl)-2,6-bis((E)-2-(thiophen-2-yl)vinyl)pyridine (**M**) (L2431) deposited by cycling (CV) or controlled potential polymerization (CPE), at different potential and charges. The increase in the peak current with concentration is more evident for CV and DPV than for RDE curves. A more in-depth study of the CV curves during the preparation of the electrode by scanning shows that the polymerization process also takes place. The CV curves obtained at variable scan rates show that all processes are irreversible in all domains. Investigation and morphological characterization of the CMEs performed using SEM, EDX, AFM, FTIR, and fluorescence methods indicated colored films obtained either by scanning or by CPE. The surface topography of organic films was investigated by AFM in scanned in contactless mode. FTIR spectra show that the organic films are thin, and the graphite substrate shields the vibrations of the bonds in the films. Transmission minima detected only on samples prepared by CPE are attributed to the presence of specific bonds. The characterization methods for CMEs were chosen depending on the desired uses of the monomers for heavy metal sensors or optical applications, respectively.

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PN2. OPTICAL AND ELECTROCHEMICAL EXPERIMENTS FOR Hg(II) ANALYSIS IN SOLUTION AND ON AZULENE-PHENYLOXAZOLONE-CMEs

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Optical and electrochemical experiments for Hg(II) analysis in solution and on chemically modified electrodes (CMEs) were performed. Novel CMEs based on several azulene-phenyloxazolones were prepared by their electrooxidation on glassy carbon in 0.1 M TBAP/ CH_3CN [1, 2] and conditioned. Then, they were used for Hg(II) ions analysis by stripping. The influence of preparation conditions (electric charge and potential) on their complexing properties was examined. This study is relevant for the design of advanced materials based on azulenyl-phenyloxazolone for the heavy metals` analysis in water samples.

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PN3. CHEMICALY MODIFIED ELECTRODES BASED ON SEVERAL AZULENYL-PHENYLOXAZOLONE FOR Cu(II) ANALYSIS

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Novel CMEs based on several azulene-phenyloxazolones were prepared by electrooxidation on glassy carbon in 0.1 M TBAP/ CH_3CN [1, 2]. After their conditioning they were used for Cu(II) ions analysis by stripping. The influence of azulene-phenyloxazolones structure on their complexing properties was examined. The detection limits of these CMEs were found and connected to the ligands structures used for their preparation. Optical and electrochemical experiments for Cu(II) analysis in solution and on chemically modified electrodes (CMEs) were performed.

[1]. A.G. Brotea, O.T. Matica, C. Musina (Borsaru), M. Cristea, A. Stefaniu, A.M. Pandele, E.M. Ungureanu, Symmetry 15 (2023) 540.
[2]. A.G. Brotea, O.T. Matica, C. Musina (Borsaru), A.M. Pandele, R. Trusca, E.M. Ungureanu, Symmetry 16 (2024) 245.

PN4. DEVELOPMENT OF SENSITIVE NANOCOMPOSITE MATERIALS FOR BIOLOGICALLY ACTIVE COMPOUNDS

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During the last decades the nanosized composite materials based on AuNPs and AgNPs, have received great interests owing to their interesting optical, electronic, thermal and catalytic properties with potential applications in the fields of chemistry, biology, physics, medicine, and material science. Their synthesis and characterization have attracted considerable attention from a fundamental and practical point of view. Thus, in the present study is described the advantage of sinusoidal current technique (SC) in the synthesis of nanocomposite materials used in epinephrine (EPI) and quercetin (QR) detection. The polymeric (PEDOT) matrix has been prepared by applying a sinusoidal current of 100 mHz frequency, I_{dc} = 25 µA, I_{sin} = 20 µA and deposition time of 300 s. This innovative method allows the synthesis of a AuNPs and AgNPs inserted in PEDOT matrix by increased electroactive area which led to the increase of sensor sensitivity. The developed sensors have been tested and validated in laboratory environment for EPI and QR determination. The analytical performance in terms of LOD, LQD and the linear range were comparable with those previously reported in the literature.

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PN5. OPTICAL EXPERIMENTS AND DFT CALCULATIONS FOR AZULENE-PHENYLOXAZOLONES

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Optical, electrochemical and quantum computed investigations based on Density Functional Theory (DFT) were conducted in order to highlight the correlation between redox potentials and predicted quantum reactivity parameters derived from energetical levels of frontier molecular orbitals. Previous works confirmed the possibility to assess electrochemical properties with good accuracy by quantum mechanical calculations using hybrid density functionals [1]. In the same manner, we used B3LYP/DFT/6- 31G (d,p) method [2] to predict quantum chemical reactivity parameters for phenyloxazolones and to correlate the calculated energies of HOMO and LUMO orbitals to oxidation, and reduction potentials, respectively. Combination of electrochemical, optical and DFT simulations allowed investigating systematically the effect of different substitution on the phenyloxazolones skeleton, that affect their properties. Several phenyloxazolones were electrochemically studied on glassy carbon in 0.1 M TBAP/ CH_3CN [3]. Studies by UV-Vis were performed for each phenyloxazolone in acetonitrile and the influence of heavy metals addition was examined to see their complexation effect.

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PN6. MODIFIED ELECTRODES BASED ON ETHENE-2,1-DIYL TETRATHIOPHENE AZULENE DERIVATIVE FOR HEAVY METALS ANALYSIS

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Based on preliminary results on the electrochemical behavior of azulene-based push-pull organic systems [1] as new materials for electrode surface modification, ethene-2,1-diyltetrathiophene azulene (L2064), has been tested to obtain modified electrodes L2064 belongs to azulene compounds, with potential nonlinear optical responses, and staining properties [2, 3].

Novel chemically modified electrodes (CMEs) based on this azulene were prepared by electrooxidation of L2064. To evaluate the chemical structure and surface images, the CMEs based on L2064 were characterized by ferrocene redox probe, X-ray photon spectroscopy, and scanning electron microscopy. They were also tested for the analysis of synthetic samples of heavy metal (HM) ions. The influence of preparation conditions (electric charge and potential) on the properties of these CMEs was examined. This study is relevant for further design and development of advanced materials based on azulenyl-phenyloxazolone for the HMs analysis in water samples.

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PN7. DETERMINATION OF EICOSAPENTANOIC ACID ETHYL ESTER IN THE LIVER OF STINGRAY

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Omega-3 fatty acids are polyunsaturated fatty acids essential for normal metabolism. Technically speaking, omega 3 fatty acids are part of the family of long-chain polyunsaturated fatty acids of carbon atoms and are represented by alpha linoleic acid (ALA), eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA). EPA can be found in stingray liver, and therefore it is essential to assay it in order to be able to know its concentrations for further processing of liver [1-3].

A cyclodextrin derivative served as modifier for the design of the modified monocrystalline synthetic diamond paste based stochastic sensor. No processing of stingray liver was necessary for the assay of EPA. Due to the biocompatibility of all components of the stochastic sensor, it can be used for in vivo measurements of EPA in the stingray liver as well, with recoveries higher than 90.00%, and %, RSD values lower than 1.00. High sensitivities and a very low determination level were obtained.

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PN8. DETERMINATION OF HUMIC ACID IN SAPROPEL USING A NEW STOCHASTIC SENSOR

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A broad spectrum of pharmacological activity of sapropel is related to humic substances: humic acid and fulvic acid being the main bioactive components. Preparations containing humic substances act at the level of non-specific and specific resistance of the organism, have antioxidant, anti-inflammatory, antiviral, antibacterial, antifungal, membrane-protecting and hepatoprotective properties [1, 2].

Conventionally it is necessary to extract the active ingredients from sapropel and after extraction to determine the humic acid content by various methods: chromatographic, spectroscopic and electrophoretic methods have been used for the analysis and characterization of humic substances [3, 4].
This paper proposed a new method for the determination of humic acid content using a stochastic sensor, a method that did not involve the extraction of active ingredients prior to the determination. The method has proven to be a very good choice for the analysis since no sample processing is needed, the sample matrix does not influence the analysis results and reliable quantitative and qualitative analyses can be performed. High sensitivity and very low limit of determination were recorded. Recoveries higher than 95.00% of humic acid, with % RSD lower than 1.00 were determined, when the stochastic sensor was used for the assay of humic acid in sapropel.

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