ICT - Interdisciplinary Smart Specialization Center in the Field of Chemical Biology, RO-OPENSCREEN

GENERAL INFORMATION

- Financing contract 371/20.07.2020, SMIS Code: 127952 concluded with the Ministry of Education and Research, as Intermediate Body for the Competitiveness Operational Programme 2014-2020 (IB COP), in the name of and for the Ministry of European Funds (MEF) as Managing Authority (MA)
- Beneficiary: "Coriolan Drăgulescu" Institute of Chemistry Timișoara (ICT)
- Project co-financed by the European Regional Development Fund through the Competitiveness Operational Programme 2014-2020
- Priority Axis 1. Research, technological development and innovation (RDI) in support of economic competitiveness and business development
- Action 1.1.1. Large R&D Infrastructures, type "Research infrastructure projects for public R&D institutions/universities – for less developed regions – LDR"
- Project duration: 20.07.2020 – 31.12.2023
- Activities: Modernization and strengthening of two buildings within ICT and equipping them with research equipment and instruments to international standards
- Total value: 42,587,899.61 lei
- Eligible non-reimbursable ERDF value: 36,090,656.29 lei

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Manager tehnic	Bora Mirela Alina
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GENERAL OBJECTIVE

The general objective of the RO-OPENSCREEN project is to increase the capacity, quality and efficiency of research-development-innovation (RDI) activity at the "Coriolan Drăgulescu" Institute of Chemistry (ICT), by creating a modern research infrastructure and equipping the newly created laboratories with high-performance research equipment and instruments, aligned with the integration requirements of the European infrastructure network EU-OPENSCREEN (European Infrastructure of Open Screening Platforms for Chemical Biology), with the aim of stimulating the competitiveness of Romanian scientific research and integrating it into the European Research Area.

SPECIFIC OBJECTIVES / EXPECTED RESULTS

- Modernization and strengthening of 2 ICT buildings currently under conservation, with the implementation of "nZEB" (nearly Zero Energy Building) energy solutions, in order to host ICT's new interdisciplinary research center, a center that will respond to international research trends and standards.

- Equipping 3 laboratories with an interdisciplinary chemical biology profile, belonging to ICT's new research center, with high-performance instruments and equipment, which will include:
  - chemoinformatics laboratory
  - chemical library laboratory
  - synthesis, analysis and structural characterization laboratories
  - sample preparation room

- Equipping with specific equipment the building serving the utilities related to ICT's new research center, with spaces configured as follows:
  - heating plant
  - reagent transfer station
  - high-performance computing system and communication system

- Construction of a library of biologically active compounds – the National Library of Biologically Active Compounds (LNCB), unique in Romania – with the aim of contributing to accelerating the drug discovery process and beyond, and of facilitating new collaboration opportunities;

- Increasing ICT's international visibility and involvement in European projects by submitting at least 3 such projects during the project sustainability period.

- Increasing the quality of human resources by developing optimal conditions for carrying out research-development-innovation (RDI) activities, maintaining the existing jobs, creating 2 new jobs, the continuous training of young researchers at doctoral/postdoctoral level, as well as attracting specialists from the diaspora are objectives to be achieved during implementation and for at least 5 years after completion of the project.

- Increasing the competitiveness of Romanian science and economy through innovation and supporting the aspiration toward excellence in frontier research through the internationalization of Romanian research, international evaluation, increasing the attractiveness of the Romanian RDI system, through mobility and public-public and public-private partnerships.

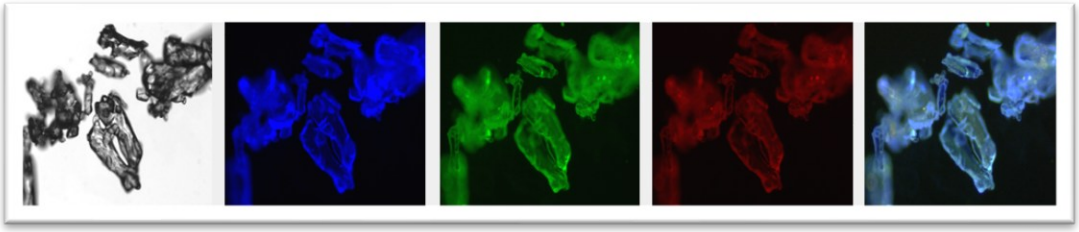
- Organizing exchanges of experience with institutions that have complementary expertise and experience, which will strengthen institutional relations and engage the associated human resources and infrastructures.

RESEARCH EQUIPMENTS

Multi-modal platform for the detection of biological activities in microplates

EVOS M7000 Microscope, Thermo Fisher Scientific

The EVOS M7000 inverted digital automatic microscope is designed for various applications in life sciences, cell biology, molecular biology and medical research.



Images of the single crystals of a multicomponent compound captured with EVOS M7000

- The microscope is equipped with:
  - 4 different objectives (4x, 10x, 20x, 40x);
  - 2 autofocus digital cameras (one monochrome and one color) for capturing fluorescence and transmitted-light images;
  - 2 phase-contrast disks for the turret condenser, useful for improving image quality in dark-field illumination of colorless and transparent samples;

- 3 fluorescence filter cubes for DAPI (357/447 nm), GFP (482/524 nm) and Texas Red (585/628 nm), making it suitable for studying the fluorescence of chemical as well as biological compounds, cellular processes, protein localization and other fluorescence-based assays;

- It automatically scans microplates and provides fast autofocus, rapid image capture and extensive data processing;
- Coupled with an incubator equipped with a gas controller (for CO2) and a temperature and relative humidity control system for monitoring living cells at different time intervals;
- The microscope supports time-lapse imaging, allowing the capture and analysis of dynamic processes over time (e.g. monitoring living cells in cell cultures).

Varioskan™ LUX Microplate Reader, Thermo Fisher Scientific

The Varioskan™ LUX microplate reader is a versatile laboratory instrument designed to perform precise and efficient measurements on microplates with multiple samples.

- It is equipped with a wide range of detection technologies:
  - UV-Vis absorbance – optical range 200–1000 nm;
  - luminescence (including BRET) – optical range 270–840 nm;
  - fluorescence (including FRET) – optical range 200–1000 nm for excitation and 270–840 nm for emission;
- Includes SkanIt™ software, which allows automation of the measurement process, facilitating the workflow with multiple samples in parallel;
- It has an integrated injection system that allows automatic distribution of reagents for optimizing rapid kinetic applications and luminescence reactions;
- Includes a gas module (CO2, O2) and temperature control for performing cell-based assays under controlled conditions.

The instrument is used for a variety of applications in scientific research: absorbance determination, fluorescence and luminescence analysis, chemical and pharmaceutical screening, cell biology analyses, kinetic analyses, enzymatic analyses, ELISA-type analyses, DNA and RNA analyses.

Automatic plate formatting/reformatting and compound aliquoting system Biomek i7 Hybrid, Beckman Coulter

Biomek i7 Hybrid (MC + Span-8) is an advanced device specialized in highly precise automatic pipetting and dispensing of liquid samples, with the capacity to handle tubes of specific sizes or microplates. This equipment can also perform plate formatting or reformatting operations, thus facilitating adaptability according to the specific requirements of experiments.

It is equipped with:

- An arm with 8 independent pipetting channels;
- An arm with a multichannel pipetting head for 96-well plates;
- 1D and 2D barcode readers;
- Device for moving plates and tip boxes across the entire work surface and in the immediate vicinity;
- Shaker compatible with laboratory equipment;
- Software for pipetting, control, integration and automation;

Biomek i7 Hybrid stands out through the optimization of reliability and operating time. Thanks to its advanced technological capabilities, this equipment establishes itself as a state-of-the-art solution for laboratory activities characterized by a high throughput level, with extensive applications in various scientific and technological fields:

- Biological and medical research: useful for preparing screening samples and the precise distribution of reagents;
- Pharmaceutical industry: it can be integrated into drug discovery processes and compound testing;
- Chemistry and materials science: facilitates the precise handling of substances;

Platform for acoustic transfer of nanovolumes Echo 650, Beckman Coulter

The Echo 650 Acoustic Liquid Handler is an advanced solution for liquid handling by means of acoustic energy. This system uses sound waves to transfer precisely sized droplets from a source to a microplate, slide or another surface suspended above the source. Through this technology, test miniaturization is facilitated and the rapid, precise and efficient handling of small volumes of liquids or chemical compounds dissolved in solvent is enabled, thus optimizing experimental resources and eliminating cross-contamination caused by the use of tips.

A distinctive aspect of the device consists in its Dynamic Fluid Analysis capability, a functionality that simplifies the experimental setup process.

The equipment provides high accuracy and repeatability of results, preserves sample integrity and viability during transfer, increases flexibility in transferring liquids to different positions and volumes, reduces operating costs by eliminating disposable tips, and reduces waste generation. This equipment will be used for the transfer of aqueous solutions/DMSO/glycerol at different concentrations, NGS reagents, culture media, primers, nucleic acids, serum, plasma, antibodies, enzymes, proteins and reagents for protein crystallography, with volumes between 2.5 nL and 5 µL depending on the solvent and transfer surface.

The platform is equipped with three different software packages for:

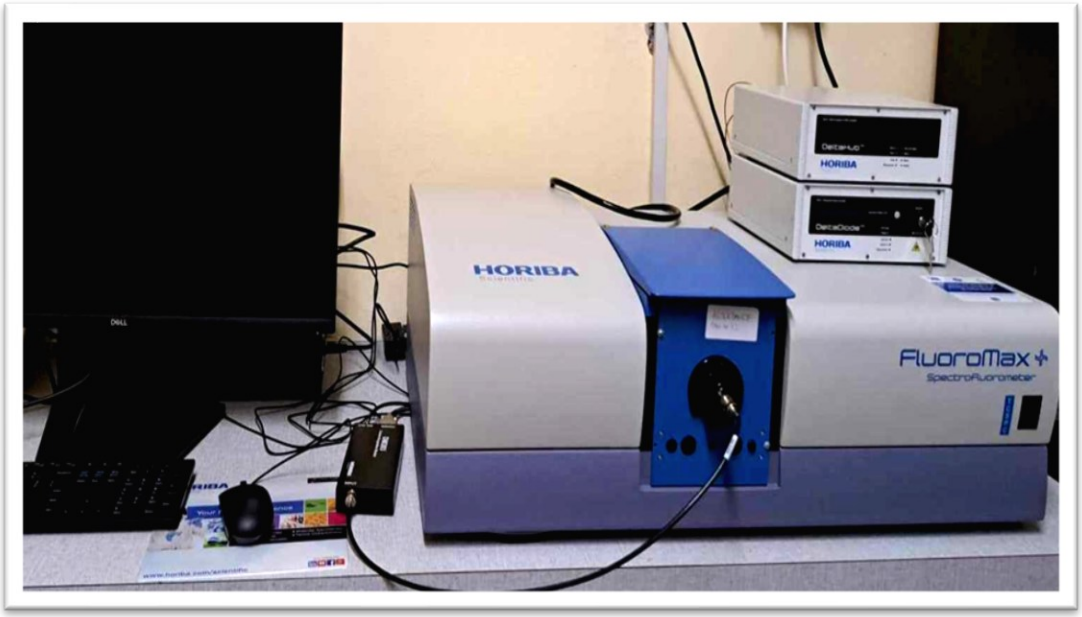
- rapid assembly or reformatting of assays (Plate reformat software);
- determination of dose-response and standard curves (Dose-response software);
- well-to-well transfer using pick-list files (Cherry Pick software);

Applications

The Echo 650 Liquid Handler is a versatile instrument, with applicability in various fields, such as drug discovery, compound management, genomic research, synthetic biology, proteomics and functional screening.

FluoroMax® Plus Fluorimeter, Horiba

FluoroMaxPlus offers a wide range of possibilities for analytical fluorescence experiments. It can measure absorbance/transmittance and fluorescence of solid, liquid and film samples, with high-speed screening, both at cryogenic and elevated temperatures. The instrument can measure anisotropies, absolute quantum yields and lifetimes by single-photon counting technique.



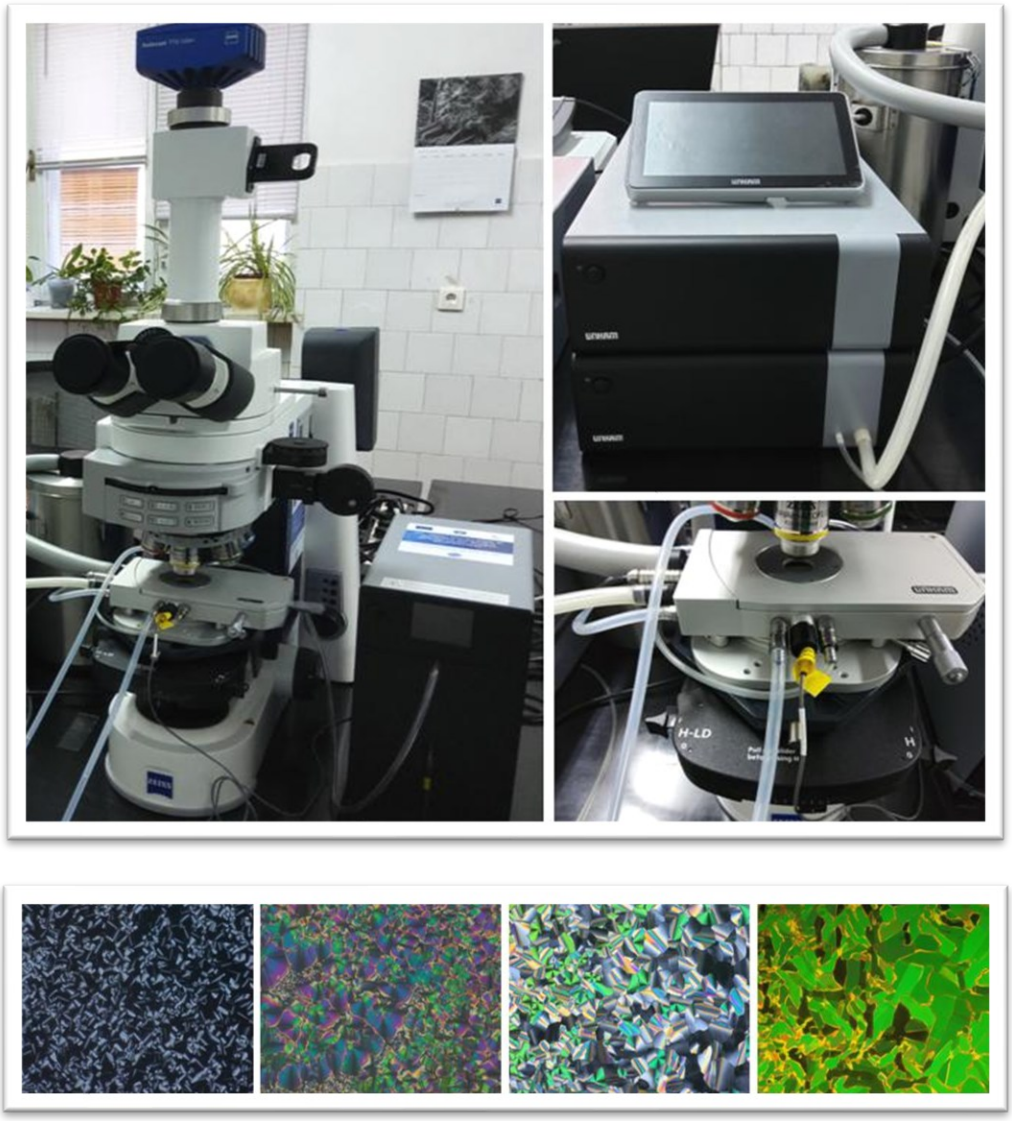
Applications:

- Analytical chemistry: determination of concentration and identification of substances in various samples;
- Nanotechnology: study of advanced materials, such as nanomaterials and nanoparticles;
- Molecular biology and biotechnology: fluorescence studies related to DNA, RNA and proteins;
- Environmental field: monitoring water quality, detecting and quantifying certain pollutants by fluorescence methods;
- Food and pharmaceutical industry: quality control of specific compounds
- Ecology: fluorescence analysis of various organisms or substances present in ecosystems;
- Optoelectronics field: photoluminescence and other optical characteristics of materials.

Polarization and fluorescence optical microscope Axio Imager A2m, Carl Zeiss Microscopy GmbH + System consisting of a heating and temperature control device for the optical microscope, Linkam

This integrated assembly between microscope and heating/cooling system provides an advanced imaging platform for the exploration and analysis of

samples in a detailed manner, under controlled cryogenic or elevated-temperature conditions.



Images of metallomesogenic compounds captured with AxioImager A2m

The AxioImager A2m microscope allows visualization and analysis of samples in transmitted and reflected light, in normal optical field but also in plane-polarized light or fluorescence emitted by samples after excitation through the Colibri system.

It is equipped with:

- 4 polarized objectives (5x, 10x, 20x, 50x);

- Polarization filters for the study of the optical properties of samples, such as anisotropy and birefringence;
- Illumination source containing 7 excitation and detection lines (UV (385nm), Violet (430nm), Blue (475nm), Cyan (511nm), Green (555nm), Yellow (590nm), Red (630nm)), which allows visualization and analysis of fluorescence in biological samples or materials;
- Software for advanced acquisition, analysis and data processing;
- Graphic workstation (PC, monitor) for equipment control, data acquisition and processing.

The AxioImager A2m microscope offers the possibility of combining techniques such as polarization and fluorescence, opening a wide range of possibilities for the exploration and detailed analysis of structures and processes at the microscopic level. The Linkam heating and cooling system provides temperature control in order to perform experiments in a thermally controlled environment and monitor them in real time.

It is equipped with:

- Thermostated chamber (min -30 °C – max 400 °C), usable for microscope slides;
- Touchscreen temperature control unit;
- Humidity controller;
- Recirculating cooling pump;
- Software for instrument control and data processing
- Graphic workstation (PC, monitor) for equipment control, data acquisition and processing;

Applications:

- Materials science: characterization of materials according to their optical, thermal and structural properties; for the study of phase transitions;
- Medicine and pharmacy: biomedical research, research in drug development and for quality control in the pharmaceutical industry;
- Cell and molecular biology: analysis of biological processes by fluorescence techniques at controlled temperatures.

The integration, by means of an optical fiber, of the FluoroMax Plus Fluorimeter with the AxioImager A2m Microscope + Linkam Heating and Cooling System, provides the possibility to carry out experiments and

analyses simultaneously, benefiting from the synergy of the information provided by the two technologies.

SAXS/WAXS X-ray diffractometer with GISAXS module, Xeuss 3.0, XENOCS

The equipment enables the determination of phase transitions in the temperature range -190°C to 350°C, the degree of ordering of materials under the influence of temperature, the degree of homogeneity of the distribution of organic groups in the case of functionalized materials, and the acquisition of structural information underlying the understanding of supramolecular architecture in the mesophase, providing information on the size, shape and distance between nanoelements, the “in situ” study of thermal stability and phase transformations for catalysts, dynamic studies as a function of temperature and humidity, the shape and size of nanoparticles, pore size and their distribution. The equipment allows adjustment of the sample-to-detector distance within the range: 50 - 1800 mm.

The equipment contains:

- X-ray diffraction diffractometer in the large-, small- and very-small-angle range equipped for measurements with the sample both in vacuum and in air;
- Detector (Dectris Eiger2R 1M);
- GISAXS and GIWAXS module;
- Sample holders for solids, liquids and powders;
- Thermostating cells with temperature control;
- Humidity and temperature control system for the sample chamber;

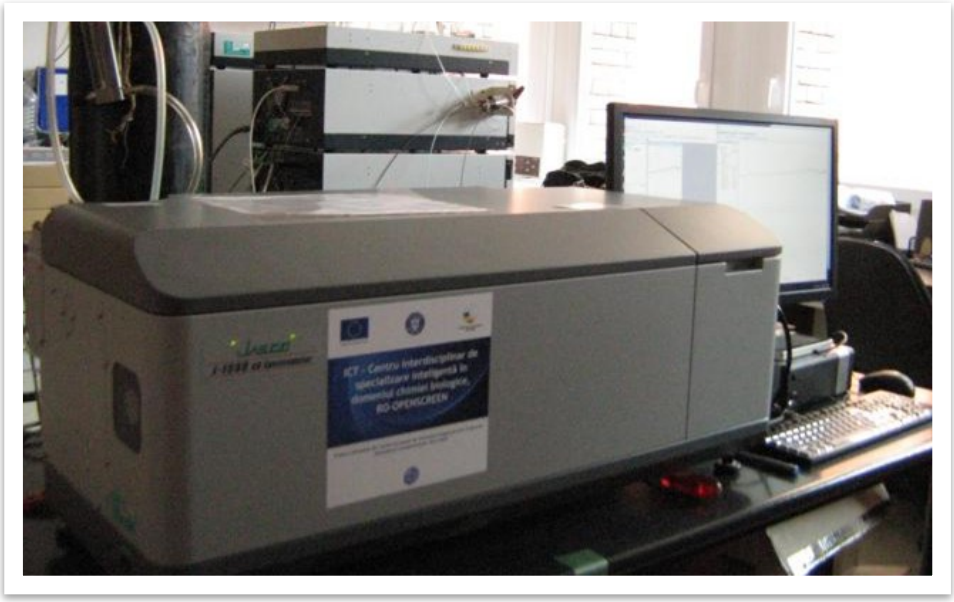
- Software for instrument control, data acquisition and processing;
- Graphic workstation (PC, monitors) for equipment control, data acquisition and processing.

Applications:

- Discovery and development of new compounds and advanced materials: characterization of crystal structures and optimization of their properties;
- Characterization of nanostructured materials: the use of the SAXS technique allows the characterization of nanostructures in solid, liquid or gaseous materials. It provides detailed information about particle sizes, shapes and distribution at the nanometric level.
- Analyses in the pharmaceutical industry: monitoring drug formulations, including the study of their nanostructure and behavior in solutions;
- Structural analysis of proteins and biomolecules: investigation of the three-dimensional structure of proteins and biomolecules;
- Research of nanomaterials and surfaces: the GISAXS and GIWAXS modules extend applications to surface studies, allowing the analysis of nanostructure at the interface of the material with the substrate or the ambient medium;
- Research of porous materials: SAXS studies are useful in the analysis of porous materials, providing information on pore distribution and pore structure in different types of materials.

J-1500 Circular Dichroism Spectrophotometer coupled with JASCO LC-4000 preparative HPLC, Jasco Inc – unique configuration in Romania

This synergistic instrument configuration is useful for the purification and structural characterization of chiral compounds that exhibit distinct optical and biological properties, the detailed investigation of material chirality as a function of temperature, and the analysis of their interactions with other molecules.



The Circular Dichroism configuration coupled with preparative HPLC contains:

- Circular dichroism spectrometer with photometric modes: circular dichroism, optical rotatory dispersion, transmittance, absorbance, HT voltage, DC voltage;
- Peltier thermostated cuvette holder and cuvettes;
- Integrating sphere (JASCO DRCD-575) with its own detector (JASCO PML-534);

- Film sample holder with temperature control;
- Optical accessory for measuring optical rotatory dispersion (JASCO ORDM-520);
- Flow cell (JASCO LCCD-420);
- Liquid chromatograph;
- Graphic workstation with operating software for equipment control, data acquisition and processing.

The liquid chromatograph allows the fractionated collection of compounds (in the milligram range) with different chirality based on the signal received from the circular dichroism detector. The adopted instrumented configuration facilitates real-time measurement of a set of significant parameters, including transmittance, absorbance, circular dichroism and pH level. These studies prove necessary for compounds that respond to the application of an external stimulus (temperature, pH, light).

Applications:

- Characterization of chiral compounds: structural characterization, including conformational analysis and enantiomer separation, with potential applications in organic synthesis, advanced materials and the pharmaceutical industry;
- Optimization of synthesis, separation and purification processes: ensures the optimization and validation of the analyzed compounds, allowing real-time monitoring of purification processes;
- Structural analysis of proteins and nucleic acid: allows the detailed investigation of the secondary structure of proteins and nucleic acid, including conformational analysis and molecular interactions;
- Detailed analysis of the components of complex mixtures: their identification and separation within preparative HPLC analyses.

Preparative liquid chromatograph C-815 Pure Flash Chromatograph, Buchi

This instrument incorporates an integrated system that combines flash and HPLC technology for the purification and separation of chemical substances from mixtures in an efficient and automated manner, through the possibility of applying positive pressure of up to 50 bar as well as a solvent gradient. These features allow the use of smaller amounts of solvent compared with classical separation methods, which reduces operating

costs. The system will be equipped with two types of detectors: the UV-Vis diode-array detector, which ensures the detection of chromophoric compounds, and the evaporative light scattering detector (ELSD) used for the analysis of compounds that do not absorb in the UV-Vis range, such as alkyl halides, sugars, fatty acids, lipids, phospholipids, polymers, surfactants, terpenoids and triglycerides. ELSD is capable of detecting all compounds that are less volatile than the mobile phase. The instrument is equipped with automatic functionalities such as: automatic sample loading, automatic fraction selection and automatic process monitoring. The flash preparative liquid chromatograph enables gram-scale mixture separations in less than 20 minutes, with improved separations compared with the classical (gravitational) method.

Applications:

- Organic chemistry: purification and separation of organic compounds, efficient separation of reaction products;
- Medicinal and pharmaceutical chemistry: purification of compounds used in drug development, separation and analysis of active substances from medicinal plants;

- Materials analysis: studies on the separation of nanoparticles and advanced materials;
- Food chemistry and food analysis: purification and separation of compounds from food;
- Chemical industry: separation and purification of chemical intermediates, synthesis and purification of compounds used in production, quality control in industrial chemical processes.

Gas chromatograph with Mass Spectrometer, Agilent Technologies

This complex configuration allows the simultaneous performance of highly sensitive qualitative and quantitative analyses, including the identification and quantification of compounds at trace level. The system is capable of separating mixtures into their individual components, identifying them and providing quantitative and qualitative information on the amount and chemical structure of each compound.

The equipment contains:

- 8890GC gas chromatograph, Agilent: ensures the efficient separation of compounds in complex mixtures;
- 7010 triple quadrupole MS/MS mass spectrometer, Agilent: offers selective detection, increased sensitivity and precise quantification capability, being ideal for the structural and quantitative analyses of chemical compounds of interest;

- 8697 Headspace module, Agilent: extends the versatility of the system by analyzing compounds in the gaseous phase, allowing the efficient analysis of volatile compounds in liquid or solid samples;
- jetClean self-cleaning ion source, Agilent: ensures consistent performance and increased reliability through periodic self-cleaning, minimizing contamination and optimizing stability over time;
- Advanced temperature control: ensures stable and reproducible conditions during analyses;
- Automatic sample injection system;
- Graphic workstation with operating software (PC, monitor) for equipment control, data acquisition and processing;

Applications:

- Medico-pharmaceutical research field: analysis of volatile organic compounds, precise identification and quantification of pharmaceutical compounds and metabolites, metabolomic and proteomic analysis regarding the composition and concentration of compounds in complex biological samples;
- Air quality monitoring: analysis of volatile organic compounds in air contributes to air quality monitoring, the identification of pollution sources and the assessment of environmental impact;
- Food safety analyses: detection of contaminants and assessment of the chemical composition of food products, ensuring compliance with safety standards;
- Environmental analysis and monitoring of hazardous chemicals: analysis of chemical compounds in the environment, including monitoring of pesticides, toxic substances and persistent organic compounds;
- Industrial analysis: quality control and production monitoring in various industries.

Vanquish Horizon UHPLC liquid chromatograph with Orbitrap IQ-X Tribrid mass spectrometer with 1M resolution, Thermo Fisher Scientific - unique configuration in Romania

This instrumental configuration is specialized in the efficient separation of compounds from complex mixtures, offering, at the same time, qualitative

and quantitative physicochemical identification capabilities based on the measurement of molecular masses at very high resolution.

The equipment contains:

- Liquid chromatograph;
- Diode-array detector;
- Mass spectrometer with a resolving power of 1,000,000 (1M – 1 million);
- MALDI ionization source (matrix-assisted laser desorption/ionization);
- Nitrogen generator with compressor;
- Graphic workstation with operating software (PC, LCD monitor) for equipment control, data acquisition and processing.

The configured liquid chromatograph allows the analysis of a wide range of compounds both at high pressure (HPLC) and at ultra-high pressure (UHPLC) up to 1500 bar, ensuring rapid and precise analyses. This liquid chromatograph ensures operation over an extended pressure range and at a reduced flow rate, for lower solvent consumption.

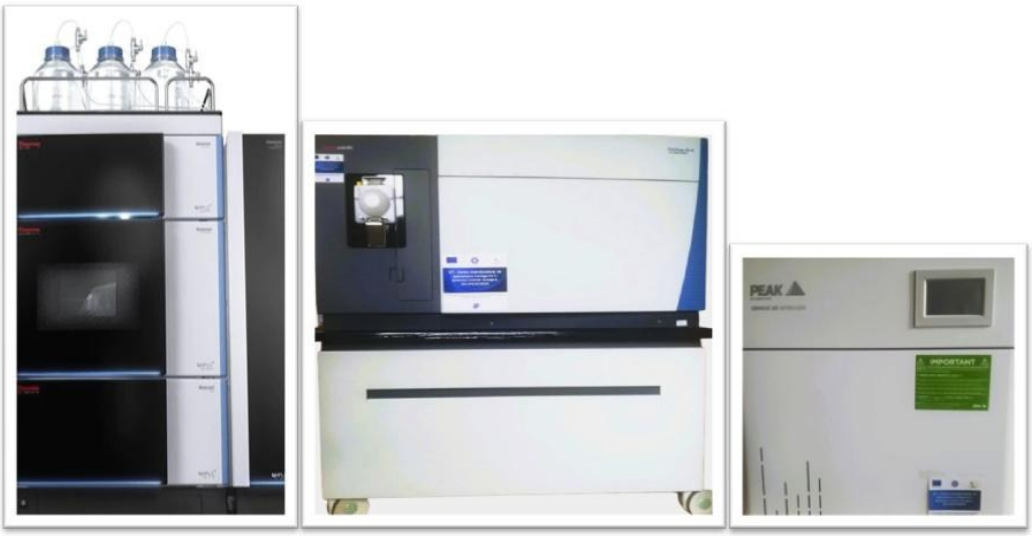
The equipment is fitted with two detectors: the diode-array detector, which ensures data acquisition over the entire UV-Vis spectrum, and the mass spectrometer, which can operate with three ionization sources (ESI, APCI, APPI), significantly extending the range of applications. For compounds with low solubility, the mass spectrometer is configured with a MALDI ionization source (matrix-assisted laser desorption/ionization) provided with a device for spraying samples deposited on TLC plates or slides.

The mass spectrometer is a state-of-the-art instrument with extensive detection and quantification capabilities at trace level. It also ensures the identification and confirmation of compounds, including those that are low-volatility, non-volatile or thermally unstable. The mass detector is one of the most advanced facilities existing in the field of mass detectors, offering the possibility of acquiring spectra for compound identification while they are quantified on the basis of the MS/MS fingerprint.

Applications:

- Advanced high-sensitivity analyses: separation and characterization of compounds from a mixture, including their identification and quantification in various samples;

- Qualitative and quantitative physicochemical identification of compounds: measurement of molecular masses with very high resolution;



- Elucidation and confirmation of low-volatility, non-volatile or thermally unstable compounds;
- Trace and minor-compound analyses: precise identification and quantification of compounds present in small amounts, including traces of substances.

Bruker-Fourier 80 FT-NMR Benchtop Spectrometer, Bruker BioSpin GmbH

This was specifically designed for use in scientific research laboratories, allowing the recording of 1D nuclear magnetic resonance spectra (1H and 13C), DEPT spectra, determination of T1 and T2 relaxation times, as well as recording of 2D spectra (COSY, JRES, HSQC, HMBC). It also offers the option of recording proton spectra in non-deuterated solvents, with solvent suppression, necessary for monitoring chemical reactions.

Applications

The equipment offers a diversity of applications in the field of organic chemistry and complex molecular analyses. In an academic context, the spectrometer proves useful in:

- Analysis of organic compounds including organic-inorganic hybrid compounds: essential information about molecular structure, electron distribution and chemical interactions at atomic level;
- Investigation of chemical bonds and molecular conformation: for understanding the properties and behavior of compounds at molecular level
- Kinetic analyses and molecular processes: provides information about reaction rates, intermediates and ongoing molecular processes.

synthWAVE semisynthesis microwave system, Milestone

This equipment uses advanced microwave technology, ensuring precise control over heating energy during chemical reactions. It has the capacity to perform parallel or serial reactions, allowing workflow optimization and increased synthesis efficiency. The system offers precise control of temperature (up to 300°C) and pressure (up to 199 bar) inside the reactor, ensuring controlled and reproducible reaction conditions. It is equipped with the advanced GoSynth™ interface, which facilitates reaction setup and monitoring.

The use of microwave technology promotes the principles of green chemistry by optimizing solvent consumption compared with traditional synthesis methods, reducing waste and saving reagents. The system has applicability in organic chemistry, biochemistry, molecular biology, materials science, the pharmaceutical industry and agrochemistry.

Applications:

- Optimization and acceleration of the synthesis of organic compounds, including stereoselective ones, efficient functionalization and derivatization, development of rapid synthetic routes;
- Synthesis of peptides and proteins;
- Synthesis of advanced materials, including nanoparticles and polymers.

UNICUBE elemental analyzer, Elementar Analysensysteme

The equipment enables the simultaneous investigation of carbon, hydrogen, nitrogen and sulfur analysis for organic, inorganic and biologically active hybrid compounds, in solid or liquid form.

The equipment contains:

- Elemental analyzer;
- Microbalance with an ultra-high degree of precision;
- Computing system;
- Instrument control software, acquisition and analysis of recorded data.

The equipment provides reliable and consistent results over a wide concentration range, for variable quantities of chemical substances, starting from 0.1 mg for solid compounds, 15 mg for liquid fuels and up to 1 g for inhomogeneous soils.

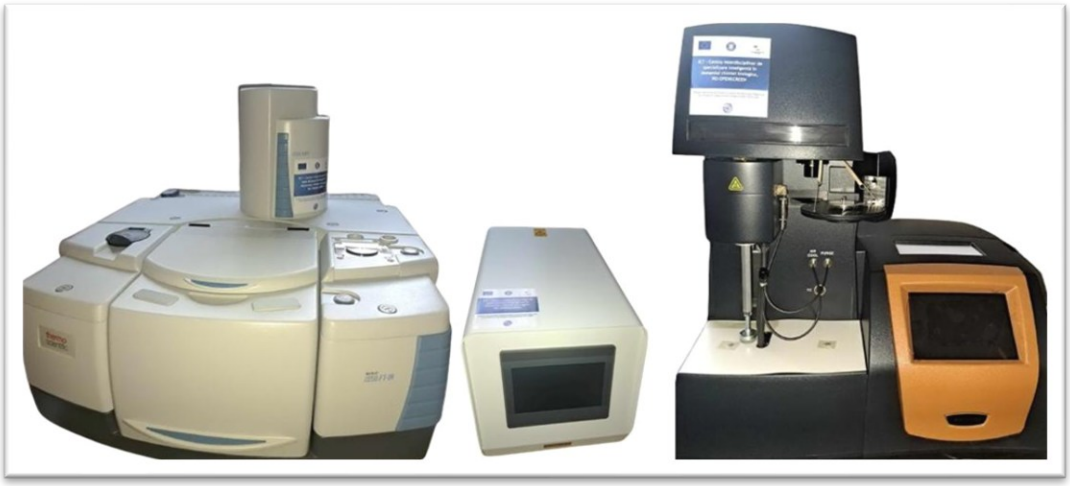
Using direct temperature programmed desorption technology (direct TPD), the analyzer chromatographically separates the gases resulting from combustion, ensuring precision in detection. The analysis is carried out by combustion at high temperatures, ensuring remarkable precision and accuracy in determining the elemental content.

Applications:

- Chemical industry: analysis of organic, inorganic compounds and raw materials used in chemical processes;
- Soil analyses: provides information about the content of essential elements in inhomogeneous soils;
- Fuel quality control;
- Pharmaceutical industry: analysis of compounds in the pharmaceutical industry, ensuring compliance with quality standards.

Discovery TGA 5500 thermogravimetric analyzer, TA Instruments + Nicolet IS-50 FT-IR Spectrometer with FT-Raman module, Thermo Scientific

The TGA analyzer allows thermal stability, decomposition kinetics, composition, estimated lifetime, oxidative stability, moisture content measurements, as well as control of the atmosphere (inert atmosphere or oxidizing conditions) in which the analysis takes place. The FT-IR spectrometer with FT-Raman module enables qualitative and quantitative spectral analyses in the NIR-MIR-FIR domain, and statistical processing of spectral acquisitions. This allows detailed investigations of chemical bonds and molecular composition in a wide range of samples. It includes an integrated diamond ATR system, for rapid and non-invasive sample analyses. The equipment can be used individually or associated via the TG-IRe RedShift coupling. Thus, the system offers the possibility of carrying out qualitative and quantitative determinations within thermogravimetric analysis, simultaneously with spectral analysis of the gases released (evolved gas analysis – EGA). This process involves the identification and determination of volatile substances, including stoichiometric analysis for processes characterized by partial mass loss, such as desolvation or decarboxylation.



The system contains:

- TGA thermogravimeter;
- TGA–IR coupling module;
- FT-IR spectrophotometer + Raman module + ATR module + purge system;

- Computing system;
- Software for the analysis, processing and advanced treatment of thermograms.

This system brings a multidisciplinary and complementary approach to the characterization of chemical compounds and materials, offering researchers and industry a versatile instrument for complex investigations.

DSC250 differential scanning calorimetry system, TA Instruments

The instrument performs measurements on thermal processes, identifying both endothermic and exothermic reactions, as well as the heat flows associated with thermal and phase transitions. Through this, parameters such as transition temperatures, melting or boiling point, crystallization time and temperature, degree of crystallinity, specific heat, oxidative and thermal stability, reaction kinetics and sample purity are determined.
The results obtained provide essential information about the behavior of a crystal, polymorphic transitions and degree of curing. Differential scanning calorimetry is useful in examining the purity and characterizing pharmaceutical compounds, liquid crystals, metals and polymers.

Applications:

- Pharmaceutical industry: study of the thermal behavior of pharmaceutical substances, including the identification and characterization of phase transitions and associated chemical reactions;
- Materials research and development (polymers, ceramics, metals, hybrid compounds): investigation of thermal behavior, including determination of transition temperatures and their thermal properties;
- Food industry: assessment of the thermal stability of foods, identification of melting and freezing points and monitoring of changes induced by thermal processing;
- Chemistry: investigation of chemical reactions and determination of reaction enthalpy
- Medicine and biotechnology: analysis of the thermal behavior of proteins, including their denaturation and thermal reactions;
- Quality control in industry: ensuring the quality of raw materials and finished products by monitoring thermal processes;

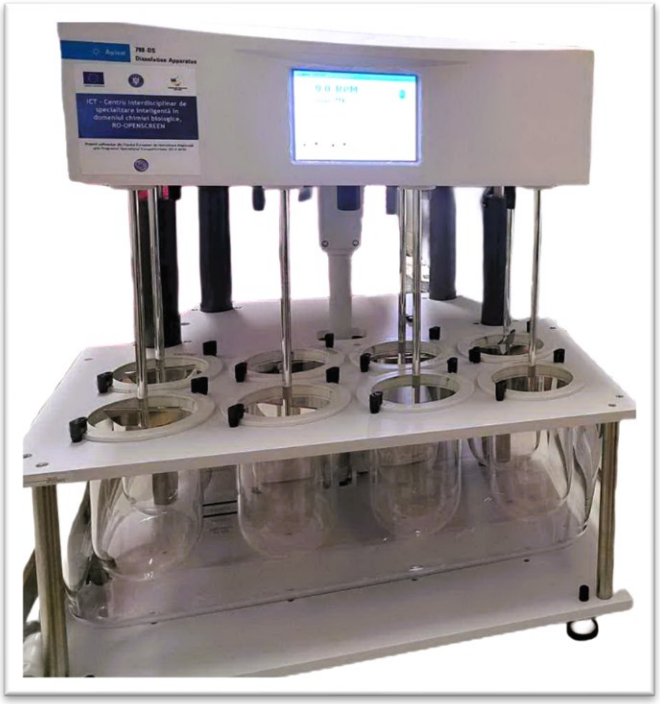
- Renewable energies: investigation of thermosensitive materials used in energy storage devices;
- Construction materials industry: evaluation of the thermal behavior of construction materials (e.g. concrete and thermal insulation);
- Stability studies in the cosmetics industry: evaluation of the thermal stability of cosmetic ingredients and finished products.

Dissolution equipment, Agilent Technologies

The dissolution equipment, consisting of the 708-DS dissolution tester and the 850-DS automated sampling system, is used in pharmaceutical and research laboratories for measuring the degree and rate of dissolution of the substance of interest (powders, tablets, capsules and even matrices that embed active substances) in liquid media. This is evaluated in media with different pH values that simulate the biological media of the body. The equipment is configured for testing in 8 positions, with baskets/paddles using 1 L vessels.

It has an advanced control system that allows monitoring and control of the dissolution process and sample collection, as well as data collection and analysis.

The equipment is a modular system designed for manual or automatic testing of sample dissolution.



708-DS dissolution tester, Agilent Technologies

850-DS automated sampling system, Agilent Technologies

Applications:

- Pharmaceutical industry/pharmaceutical research and development: evaluation of the solubility of active substances, as well as testing of pharmaceutical formulations in different solvents and environmental conditions;
- Quality control: monitoring the quality of pharmaceutical products;
- Chemistry and biochemistry: evaluation of the dissolution process of new substances under different conditions;
- Food industry: evaluation of the dissolution process of food ingredients in different media, contributing to the optimization of production processes;
- Medical device industry: evaluation of the dissolution behavior of the materials used in the manufacture of these devices.

FreeZone Plus 4.5 L Cascade Benchtop sample drying system, Labconco

The equipment is used for drying samples (synthesis compounds or biological samples) before analyses and subsequent characterization. The system uses a technology involving several cooling stages to ensure efficient and rapid drying of samples. It is connected to a scroll vacuum pump, manufactured by Edwards. The equipment includes an automatic detection kit for the end point of sample lyophilization for 2 sample vessels simultaneously, a lyo chamber with lid, chemically resistant, made of stainless steel with Teflon-coated interior, as well as a transparent lyo chamber made of acrylic material, both having ports that allow the connection of both ground-neck flasks and beaker-type vessels.

Applications:

- Chemistry: rapid and efficient drying of solvents;
- Molecular biology and biotechnology: useful in nucleic acid purification processes;
- Pharmaceutical industry: drying of pharmaceutical samples under controlled conditions (e.g. active substances or intermediate products);
- Food industry: drying and preparation of food samples for laboratory analyses or for their preservation;
- Nanotechnology: drying of nanostructured materials or nanocomposites under controlled conditions to preserve their properties;

- Electronics industry: drying of electronic components or equipment sensitive to humidity in order to prevent their deterioration.

Sample drying system, Labconco

TSGP10 bead bath, Thermo Fisher Scientific

The equipment ensures the heating and constant maintenance of the temperature of samples/compounds during experiments/tests and provides uniform heat distribution around the container.

Ghibli Pro sample drying chamber - 350L, Ghibli Pro

The equipment allows the drying or processing of samples in a controlled and controllable environment. Useful in various scientific research fields (chemistry, medicine)/industries (chemical, pharmaceutical, food, textile, electronics). It is provided with a portable hygrometer with LCD screen for optimal control of humidity and internal temperature, programmable timer, parameter monitoring systems as well as internal lighting.

TSGP10 bead bath
Thermo Fisher Scientific

350L sample drying chamber,
Ghibli Pro

IC0105 Incubator, Memmert GmbH

The equipment allows precise control of temperature and humidity, as well as uniform heat distribution in the working chamber, through easy programming. It is frequently used in research laboratories for the cultivation and incubation of cell cultures/microorganisms/biomedical samples, but also for the storage and maintenance of biological or chemical samples under controlled conditions.

IC0105 Incubator, Memmert GmbH

Solvent trapping system for high-vacuum pump WCT-80, Witeg Labortechnik

The equipment is used for capturing and recovering volatile solvents and vapors released during work processes. It has a cooling bath and 2 solvent trapping vessels with pressure and temperature resistance, which ensure efficient condensation and collection of solvent vapors from the working space.

Applications:

- Chemistry: collection of volatile solvents resulting during chemical reactions sensitive to solvents;
- Pharmaceutical industry: collection of solvents used in the synthesis processes of active pharmaceutical substances;
- Analytical chemistry: collection of solvents used in different analytical techniques, such as liquid chromatography or gas chromatography;
- Paints and varnishes industry: solvent capture in manufacturing processes and compliance with environmental standards.

SL8R refrigerated centrifuge with swing-out rotor, Thermo Fisher Scientific

The equipment has a modular design that allows rapid switching between rotors intended for microplates and angled tubes, thus offering versatility in centrifugation processes. It is equipped with an advanced cooling system to maintain optimal temperatures during centrifugation, ensuring sample stability and preventing their degradation. The swing-out rotor allows easy loading and unloading of samples, facilitating handling and minimizing preparation time.

Applications:

- Molecular biology and biotechnology: DNA and RNA purification, as well as cell separation;
- Cell biology and immunology: separation of cellular components;
- Medicine: clinical analyses and diagnostics, as well as for the separation and preparation of samples for mass spectrometry, chromatography and other analytical techniques;

- Pharmaceutical industry: separation and purification of pharmaceutical substances, including proteins and other biotechnological products;
- Environmental science: analysis of water and sediments;
- Food production and quality control: evaluation of food composition and properties, including analyses of fat, proteins and contaminants;

- Materials science: separation of the liquid phase from complex materials;
- Chemical and petrochemical industry: quality control and analyses of chemical processes, including the separation and identification of chemical substances.

Forced-convection (mechanical) oven SLW 53 IG Smart, Pol-Eko

The oven is equipped with a digital control system that allows precise setting of temperature and operating time and has functions for monitoring operating parameters. It ensures the hot-air sterilization of large objects made of thermally resistant materials.

Horizontal autoclave with drying ST DRY PV -B 23L, J.P. Selecta

The autoclave allows steam sterilization under pressure of small objects (laboratory instruments, culture media, medical instruments, packaging materials, biological materials). The autoclave is equipped with a drying function, efficiently removing moisture from sterilized materials. It has a digital control system that allows the precise programming and monitoring of sterilization parameters, such as temperature, pressure and time.

Forced-convection oven
SLW 53 IG Smart, Pol-Eko

Horizontal autoclave with drying
ST DRY PV -B 23L, J.P. Selecta

High-speed tube opener LABELITE, Hamilton

The equipment offers high operating speed, advanced automation, compatibility with various types of tubes, as well as precise control of tube opening, thus minimizing the risk of contamination. It can be operated as a stand-alone device or integrated with a liquid handling system or a third-party robotic arm. The advantage of using an automatic decapper is increased work efficiency and reduced injuries caused by manual decapping. The purchased equipment allows individual selection of tubes, which helps minimize contamination caused by decapping unnecessary tubes.

Applications

Applicable in the field of life sciences, pharmaceutical industry, for use in:

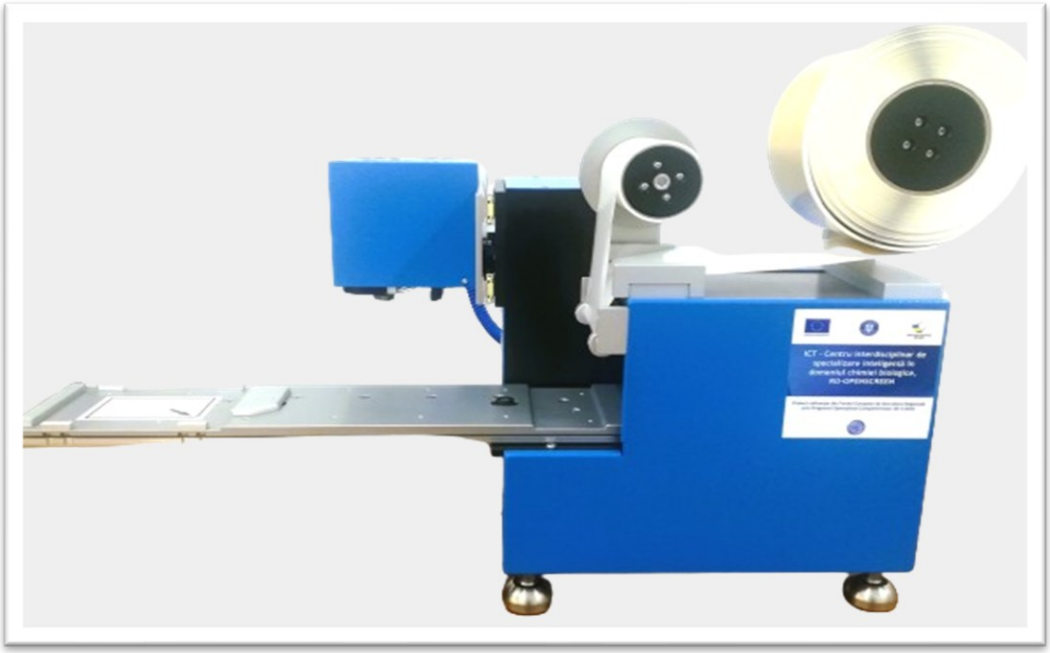
- automation of screening processes involving the handling of a large number of samples in a short time
- opening of tubes used in biotechnological processes, including molecular biology analyses, proteomic analyses or genetic studies.

Thermostated plate shaker CRPI-412X, CAPP/AHN Biotechnologie

The equipment offers various functions: shaking, simultaneous heating of plates, precise temperature control, capacity to operate with 4 plates simultaneously in order to increase process efficiency and allow parallel analyses, variable shaking speed, as well as temperature uniformity in all 4 plate positions.
It is applicable in biology, medicine, pharmacology and chemistry, being used for the growth and cultivation of cells, cell cultures, screening of chemical substances and drugs, enzymatic analyses, growth and study of microorganisms, bacteria and fungi, immunological and serological analyses, DNA amplification and other genomic techniques.

Automatic station for plate sealing and unsealing HJ@SealPeelStation, HJ-BIOANALYTIK GmbH

The equipment provides automatic plate recognition both in the sealing and unsealing process and allows the application and removal of films from plates. The fixing and sealing of the adhesive film is achieved only by pressure, eliminating the disadvantages caused by heat or the problems caused by inadequate adhesion between film and plate.



96-well plate washer 50 TS8, BioTek Agilent Technologies Inc

The equipment allows washing of 96-well plates, as well as individual washing of 8-well rows. It is equipped with a programmable control system, allowing the configuration and programming of different washing cycles according to the specific requirements of the experiment. It has pressure and liquid-volume control functions for each washing stage, as well as a precise dispensing system, which allows accurate dosing of the washing liquids into each well.

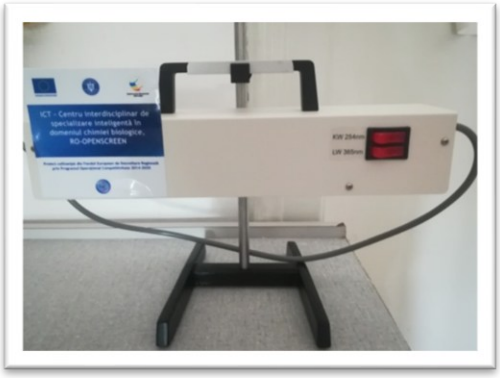
Applications

It is applicable in medicine, the pharmaceutical industry and chemical research, being used for:

- efficient washing of plates used in immunological analyses, molecular biology, chemical compound screening.

Ultraviolet lamps

UV lamps are equipment used for the identification and highlighting of compounds that exhibit UV absorption or fluorescence. The wavelength of 254 nm is used for visualizing the plates used in thin-layer chromatography for reaction monitoring, while the wavelength of 365 nm is useful both for observing fluorescence and in polymerization reactions using photoinitiators.



UV lamp 8W, Herolab

UV lamp 15W, Vilber

Calcination furnace L9/11, Nabertherm

The equipment is specialized in the calcination process, which involves heating a wide range of materials at high temperatures (up to 1100°C with a maximum variation of ±5°C) to change their chemical or physical properties. The furnace offers applicability in different industries (ceramics, glass, metallurgy) and scientific fields (chemistry, electronics, catalysts).

Recirculating cooling equipment

This equipment is essential in research laboratories and industry, offering precise temperature control in applications that require a high cooling capacity, as well as efficient mild-condition condensation of solvent vapors. Rotary evaporators, autoclaves, reaction vessels, Soxhlet apparatus or vacuum systems are applications that require constant and reproducible cooling conditions. Recirculating cooling equipment operates with universal coolants (methanol, ethanol, glycol), under pressure, and supplies a coolant flow at controlled temperature. The dual cooling equipment has two cooling cycles directly connected to the double outlets and inlets, which offers the possibility of connecting two applications in parallel, thus optimizing laboratory workflows.

Single cooling equipment
F250 JULABO, GmbH

Dual cooling equipment
RC-10 Duo, VWR

Vacuum oven SWOV 30, WITEG Labortechnik GmbH

The equipment allows the drying/treatment of samples under vacuum conditions. The integrated vacuum system and temperature controller create a temperature-controlled environment under reduced pressure that improves sample drying conditions. It is used in both research and industry for drying or treatment processes that require vacuum conditions.

Ice flake equipment M-ICE 50, Maxima

The equipment supplies ice in the form of flakes, useful in laboratory or industrial processes that require ensuring the proper cooling of chemical syntheses and/or the reaction medium.

Rotary evaporator with vacuum pump HEI-VAP EXPERT, Heidolph Instruments

The equipment is used in laboratories from different scientific and industrial fields for the separation and concentration of chemical substances from a liquid. It has a rotary evaporation system, heating bath with a precise temperature and rotation speed control system, and chemically resistant vacuum system.

Vacuum pumps

Vacuum pump for oven PC 611 select, Vacuubrand GMBH

It can be used in chemistry laboratories for the oven with vacuum system, for drying temperature-sensitive samples without damaging them, as well as for the simultaneous processing of compounds obtained by other methods that require vacuum.

Advanced vacuum pump RC6, Vacuubrand GMBH

It can be used in chemistry laboratories for the freeze-dry technique for processing organic, inorganic and biologically active compounds.

Vacuum pump for oven PC 611 select, Vacuubrand GMBH

Advanced vacuum pump RC6, Vacuubrand GMBH

Magnetic stirrer with cooling for low-temperature syntheses LSRB-8002, LABFREEZ INSTRUMENTS

The equipment allows the maintenance of low temperatures (down to -80°C) during longer synthesis processes, as well as precise temperature control. It has magnetic stirring to ensure homogeneous mixing of substances during synthesis. The equipment can be used in both research and industry for the synthesis of chemical compounds or studies on materials at low temperatures.

Laboratory conductivity meter S230-B, SEVENCOMPACT

The conductivity meter allows the measurement of the electrical conductivity of solutions, providing information about:

- the content of salts and ionic substances in a solution
- the behavior of ionic compounds in aqueous solutions with biological relevance

- the quality of water (water with a certain maximum conductivity value depending on use) used in the processes of characterization, synthesis or processing of chemical compounds

Laboratory pH meter, HANNA

The equipment allows the measurement of the concentration of hydrogen ions (pH) in water-based solutions, indicating the acidity or alkalinity of a substance.

The equipment can be used for:

- measuring pH in chemical solutions and for identifying the acidic or alkaline nature of substances;
- soil monitoring;
- checking drinking water quality;
- monitoring and controlling pH in various chemical and industrial processes.

Ultrasonic bath Elmasonic S30H, Elma Schmidbauer

The equipment allows use in:

- scientific laboratories for mixing, dispersion, emulsification, dissolution and/or degassing of samples, but also for cleaning laboratory instruments made of glass, plastic or metal;
- various industries (electronics, automotive, metallurgy, food) for cleaning and degreasing the components/objects used.

Analytical balances

The equipment is precision instruments used for the exact measurement of small quantities of substances with an accuracy of up to 5 decimal places. They are used in research laboratories, pharmaceutical, food, chemical industries and in other fields where precision is essential (e.g. preparation of standard solutions).

Analytical balance with 5 decimal places AS82/220.X2 PLUS, Radwag

Analytical balance with 4 decimal places AS 520.R2 PLUS, Radwag

Analytical balance with 2 decimal places, WLC 1/A2/C/2, Radwag

Magnetic stirrers with heating and heating mantle, Hei-PLATE Mix 'n' Heat Core, Heidolph

This laboratory equipment uses a rotating magnetic field to mix liquids and homogenize them. The rotating magnetic field can be generated by a rotating magnet or by a set of stationary electromagnets, placed under the liquid vessel.

Applications

They will be used for stirring solutions in open or closed systems, under inert atmosphere, in laboratory operations such as organic and inorganic synthesis, pH measurements, preparation of buffer solutions. They offer advantages compared with geared motorized stirrers, because they are quieter, more efficient, can also be used for closed systems, and have no external moving parts that can break or wear out.

Dewar vessel for the transport and storage of liquid nitrogen 35LDB, IC Biomedical

The Dewar vessel is a thermally insulated container used for the storage and transport of liquid nitrogen at atmospheric pressure, of other cryogenic liquids or of substances at low temperatures. It is used in various fields such as scientific research, laboratory industry, medicine, pharmaceutical, food, and aerospace industry, for:

- the storage and handling of liquid nitrogen, allowing extreme temperatures to be maintained for long periods of time;
- the storage of biological samples (cells or tissues) at very low temperatures, keeping them viable for medical use or in research;
- the storage and transport of samples and chemical/food substances at cryogenic temperatures.

Liquid nitrogen generator Triton2s Plus, Noblegen

The liquid nitrogen generator is an efficient and reliable cryogenic solution. It is used for various applications where very low temperatures or a large temperature reduction are required, such as: NMR spectroscopy, cryopreservation, cryotherapy, gastronomy, in vitro fertilization, two-dimensional gas chromatography, dermatology, treatment of metals in order to improve physical properties, etc.

Dewar vessel
35LDB, IC Biomedical

Liquid nitrogen generator
Triton2s Plus, Noblegen

Portable cooling system, Vevor

The equipment allows the easy transport of plates with chemical compounds and of various materials (analysis reagents, chemical compounds, culture media).

Portable incubator ICT-P, FALC Instruments

The equipment allows the easy transport and maintenance of biological samples under controlled temperature conditions with an accuracy of ± 0.1°C at 37 °C. It has a temperature monitoring and display system, digital control for temperature setting, as well as a mains power supply and a car cigarette lighter socket.

Water purification systems

Crystal 7 pure series deionizing distiller, Adrona SIA

The equipment allows the production of purified water, free of mineral salts, impurities and ionic particles, optimal for use as solvent for chemical syntheses and glassware rinsing.

Smart2Pure 3 UV/UF water ultrap purification system, Thermo Scientific

The equipment allows the production of type I and II ultrapure and pure water that can be used in molecular biology and microbiology applications (PCR, cell and tissue cultures, etc.), analytical chemistry (HPLC, GC, GC-MS, etc.) or for routine laboratory applications (preparation or dilution of reagents and solutions, feeding autoclaves, rinsing glassware, etc.).

Deionizing distiller
Crystal 7 pure series

Water ultrap purification system
Smart2Pure, 3 UV/UF

Barcode printer i3300, Brady, and barcode readers Gryphon I GBT4500 /WLC4090, Datalogic

This equipment allows the printing of barcode labels required for labeling microplates, tubes, labels or containers for compound storage, as well as the scanning of 1D and 2D barcodes for the rapid identification and monitoring of compounds/samples.

Refrigeration systems

Ultra-low freezer TSX40086V, Thermo Fisher Scientific

The equipment uses advanced technologies for efficient and uniform refrigeration and maintenance at very low temperatures (down to -80ºC) of reagents, compounds in solid or liquid state, as well as biological samples. It is essential in various fields, including scientific research as well as in the pharmaceutical and food industries.

Laboratory freezers and refrigerators, Liebherr

This equipment allows the storage and preservation of chemical substances/biological testing kits under optimal conditions, in an environment protected from light, dry and cool.

Ultra-low freezer TSX40086V
Thermo Fisher Scientific

Laboratory Refrigerator / Freezer
Liebherr SRFvg 4001/SFFvg 4001

IT AND COMMUNICATION EQUIPMENT

High-performance computing system

The configured high-performance computing system allows the processing of large amounts of data and the performance of complex calculations in a short time due to the combination of several high-speed processors and large-capacity RAM, which allow the simultaneous accomplishment of tasks. The parallel data storage system allows them to be distributed over several hard disks, increasing data access speed.
The capabilities of the high-speed and high-efficiency processing system allow its use in carrying out research activities, bioinformatics, visualization or analysis of large amounts of data, etc.

Configuration of the computing and data storage system:

Computing system - GPU Server 4U

Lenovo ThinkSystem SR860 V2 – 6 nodes

- 1 GPU NVIDIA A30 24GB PCIe Gen4 Passive GPU
- 4 CPUs Intel Xeon Gold 5318H 18C 150W 2.5GHz, RAM memory 64 GB (16GB DDR4 3200 MHz)
- 6 GPUs NVIDIA 6*24GB, 432 cores/864 threads, memory 384 GB

Data storage system

- 1 IBM FlashSystem 7300, memory 768GB RAM

Graphic workstations

- Processor: IntelCore i9 12900k
- SSD storage capacity: 1TB
- Memory capacity: 32GB RAM DDR5
- Video card: nVidia RTX A2000, memory 12GB

- The graphic workstations offer outstanding advantages through increased working speed and the substantial reduction of the time required for advanced theoretical calculations.

SOFTWARE APPLICATIONS

Gaussian 16

GaussView 6

Schrödinger

Chemaxon

REACTOR

SIMCA 18

SciFinder®

The choice for chemistry research.™

CCDC the Cambridge Structural Database (CSD)

OriginPro

ChemDraw

CorelDRAW®

NATIONAL LIBRARY OF BIOLOGICALLY ACTIVE COMPOUNDS (LNCB)

Unique in Romania

LNCB - the first technology and expertise platform in Romania for chemical biology.

The main objective pursued is the construction of a highest-quality library in order to accelerate the drug discovery process and beyond.

In 2023, the LNCB library comprises 6,292 compounds, of which 2,692 are approved drugs and natural compounds and 3,600 are diversity compounds.

LNCB will be continuously enriched with an increasing number of compounds collected from the Romanian synthetic chemistry community, as a broad collaborative effort towards achieving the common objective of building a highest-quality library of biologically active compounds aligned with international trends.

The compounds collected from the Romanian chemistry community will be stored and managed at the RO-OPENSCREEN interdisciplinary center, Timișoara.
The integrated research infrastructure will allow automatic management of the compound library, extensive physicochemical investigations (e.g. solubility, ROS, etc.) and complete analytical services for the characterization of the structure of chemical compounds according to approved European procedures. The compounds thus prepared will be subjected to biological tests carried out in collaboration with specialists from Romania and Europe.

LNCB represents a key resource of chemical information for researchers from many fields of biomedical science, including chemistry, chemical biology and medicinal chemistry, and bioinformatic/chemoinformatic fields, etc.

LNCB – "open access" resource *Access to LNCB resources is open ("open access") to all academic research institutions, universities, pharmaceutical industry, chemical industry, etc., interested in cooperating and contributing to scientific excellence.*

PROJECT INDICATORS

Pre-established indicators	Approved value	Achieved value
Pre-established result indicators		
3S44 - Public-private scientific co-publications	1	1
Pre-established output indicators		
CO24 - Research, innovation: Number of new researchers in the entities that benefit from support	2	2.21
CO25 - Research, innovation: Number of researchers working in improved research infrastructures	3	5.33
Additional indicators		
Additional result indicators		
Number of project proposals submitted for other international research programmes (number)	3	6
Additional output indicators		
New R&D laboratories created through the project (number)	3	3
New jobs created, other than for researchers, in the supported entity (number)	2	3
Tangible assets acquired (pieces)	146	146
Intangible assets acquired (pieces)	37	37
Modernized area (sqm)	328	328

REHABILITATION OF BUILDINGS

INTERDISCIPLINARY CENTER - RO-OPENSCREEN

RO OPENSCREEN

Interdisciplinary Center - RO-OPENSCREEN

- ***The modern infrastructure of the interdisciplinary center opens the possibility for the development of new research directions, the training of new specialists and the development of collaborations with research institutions, universities, industry and economic agents.***

- ***The National Library of Biologically Active Compounds (LNCB), unique in Romania - an "open-access" resource.***
  Synthetic chemists in Romania are invited to deposit compounds in the LNCB in order to create a resource of chemical compounds that can be evaluated for biological activity!

- ***The interdisciplinary center offers an attractive, stable and performance-oriented framework for young researchers who wish to develop a professional career in the field of chemical biology.***

- ***This large-scale initiative contributes to the development of the capacity, quality and efficiency of scientific activity at institutional, regional and national level, with the aim of including Romania as a full member in the European EU-OPENSCREEN network, as well as initiating and carrying out national or European projects with major scientific and social impact.***

- ***Through the implementation of the RO-OPENSCREEN project, ICT has become a POLE of interdisciplinary scientific excellence aligned with the new international research trends and standards in the field of chemical biology.***

RO OPENSCREEN

THE MISSION of the "Coriolan Drăgulescu" Institute of Chemistry

The "Coriolan Drăgulescu" Institute of Chemistry (ICT) of the Romanian Academy has a tradition of more than fifty years in fundamental research in the field of organic, inorganic and theoretical chemistry.

Following national, European and international trends in scientific research, development, innovation and technological trends, ICT has directed its main research activities toward the computational design, synthesis and characterization of environmentally friendly and pharmaceutically active compounds with applications in environmental protection, the biomedical field, pharmacology and medicine.

ICT's experience and expertise focus mainly on the development of:

- new multifunctional compounds (e.g.: complex combinations of d-block metals, organic compounds that react under the action of external stimuli, etc.) with relevance in nanostructured materials science, biochemistry or environmental protection;
- new multifunctional organic and polymeric compounds containing heteroelements with targeted properties and having applications in environmental protection and sustainable development;
- advanced multifunctional materials with special optoelectronic properties based on porphyrins and their complex combinations, with biological and technical applications;
- new algorithmic techniques for the study of compounds with biological activity, chemoinformatic applications and computational techniques to develop new compounds with potential agrochemical activity, repurposing of approved drugs, collection and management of compound libraries, etc.

In order to achieve the ideal of excellence in research, the Institute's strategic objectives also target performance in the education, specialization and promotion of human resources, with emphasis on supporting young researchers and encouraging them to undertake training and documentation stages (doctorate, post-doctorate, etc.).

ICT organizes annually the scientific event “New Trends in Chemistry Research”, which reached its 15th edition in 2023 - www.newtrends-timisoara.ro/, and which, through the high quality and diversity of the scientific programme carried out, the scientific information presented, the research equipment promoted and the open discussions regarding ongoing studies and career-development studies, supports and contributes to the progress of young researchers and adds value to research activities by contributing to knowledge of the latest trends in the field.

The need to develop and maintain ICT’s research infrastructure in working condition has prompted the Institute’s researchers to access competitive funding (UEFISCDI competitions, European competitions: HORIZON 2020, etc.), resulting in the percentage increase of funding from alternative sources to those provided from the state budget through the Romanian Academy (the main funding source), and at the same time in the modernization, strengthening of excellence and increase of scientific relevance.

Through the RO-OPENSCREEN interdisciplinary center, ICT offers, as a main advantage, access to the high-performance infrastructure and the resources of the National Library of Biologically Active Compounds (LNCB) for all research institutions, universities and pharmaceutical industry interested in cooperation.

The Institute’s research programme offers the perfect framework to continue current research at a higher level and to create new research directions, to increase the education and specialization of human resources, to facilitate knowledge exchange within the scientific community and to establish new cooperation at national and international level.