



UNIUNEA EUROPEANĂ



Instrumente Structurale  
2014-2020

# **RO-OPENSREEN**

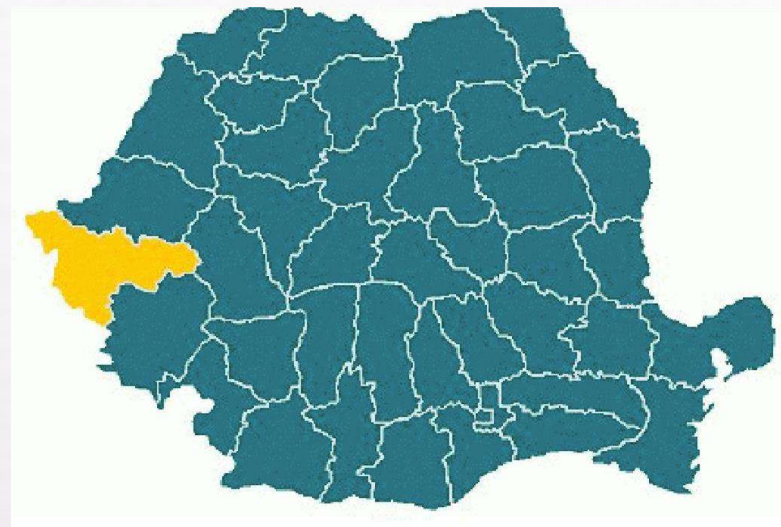
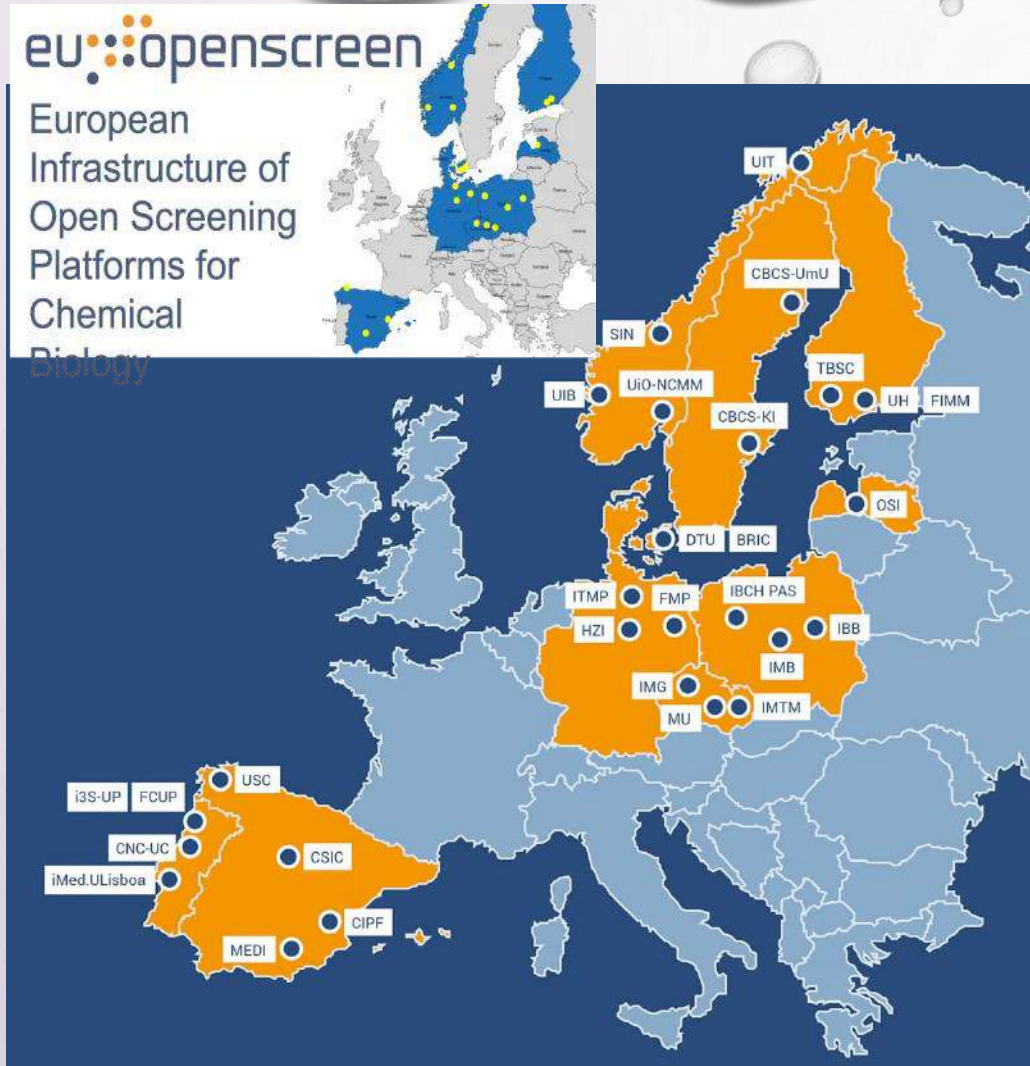
## **ICT - Interdisciplinary Center for Smart Specialization in Chemical Biology**

**Liliana CSEH, Manuela CRISAN, Alina BORA**

*"Coriolan Dragulescu" Institute of Chemistry, 24 M. Viteazu Av., 300223, Timișoara, Romania*



eu:openscreen  
European  
Infrastructure of  
Open Screening  
Platforms for  
Chemical  
Biology



**RO-OPENSSCREEN**  
**ICT - Interdisciplinary Center for  
Smart Specialization in Chemical  
Biology**

# OUTLINES

- ❑ GENERAL INFORMATIONS
- ❑ GENERAL / SPECIFIC OBJECTIVES
- ❑ EXPECTED RESULTS
- ❑ THE CURRENT STAGE OF THE PROJECT ACTIVITIES IMPLEMENTATION
- ❑ THE PROJECT TEAM
- ❑ CONCLUSIONS / TAKE HOME MESSAGE...

# GENERAL INFORMATIONS

❑ **Project title:** *ICT - interdisciplinary center for smart specialization in the field of chemical biology,*

## *RO-OPENSREEN*

❑ **Beneficiary:** “Coriolan Dragulescu” Institute of Chemistry – (ICT), Timișoara

❑ **Program:** *Competitiveness Operational Program (POC) 2014-2020; Priority Axis 1* – Research, Technological Development and Innovation to Support Economic Competitiveness and Business Development; *Investment priority 1a* – Improving research and innovation infrastructures and capacities to develop excellence in RDI and promoting centers of expertise, especially those of European interest; **Action 1.1.1** Large research and development infrastructures

❑ **Project duration:** 20.07.2020 – 31.12.2023

❑ **MySMIS Code:** 127952

❑ **Total Investment Value:** 42,587,899.61 RON

❑ **Project financed by:**

● **European Regional Development Fund (ERDF):** 36 090 656 79 RON

## GENERAL OBJECTIVE

- of the **RO-OPENSSCREEN project** is to increase the capacity, quality, and efficiency of the research-development-innovation (**RDI**) activity of the "Coriolan Drăgulescu" Institute of Chemistry (ICT), **by creating a modern research infrastructure** and equipping the newly created laboratories of the *Interdisciplinary Center for Smart Specialization in Chemical Biology, RO-OPENSSCREEN* with high-performance research equipment and tools, **aligned to the European infrastructure network EU-OPENSSCREEN** (*European Infrastructure of Open Screening Platforms for Chemical Biology*) in order to stimulate the competitiveness of the Romanian scientific research and its integration in the European research space.

The Center will carry out integrative research by applying advanced technologies of automated management of compound libraries, chemical synthesis, structural analysis, determination of biological activities and chemoinformatics.

## SPECIFIC OBJECTIVES

- ❑ Development of *the new ICT interdisciplinary research center, RO-OPENSREEN*, by modernizing/consolidating two buildings and equipping them with state-of-the-art research equipment.
- ❑ Implementation of the High-throughput screening (HTS) technology, in a systematic and automatic modes, of chemical compounds from the newly created chemical library, *the National Library of Biological Active Compounds (LNCB)*, and optimization of the compounds physico-chemical properties in order to develop tool compounds that can be transformed into products for use in related fields.
- ❑ Increasing *Romanian science's international visibility and competitiveness* by involving ICT in European projects, and public-public and public-private partnerships.
- ❑ *Increasing the quality of human resources* by developing the optimal conditions for CDI activities, *maintaining existing jobs and creating new ones, training young researchers* at the doctoral/postdoctoral level, and *attracting specialists* from the diaspora.
- ❑ Organizing *exchanges of experience* with institutions that present expertise and complementary experience will strengthen institutional relations and train existing human resources and infrastructures.

## EXPECTED RESULTS

- ❑ **Modernization/consolidation of two** of our own buildings under conservation, namely **C20** and **C21**.
- ❑ **The new ICT interdisciplinary research center**, will ensure the functionality of the following:
  - C21 building:**
    - Chemoinformatics laboratory
    - Chemical bookstore laboratory
    - Chemical synthesis, characterization and analysis laboratories
  - C20 building:**
    - Thermal power plant
    - Reagent transfer station
    - IT (cluster) and communication systems
- ❑ To complement the existing ICT infrastructure by modernizing and equipping the laboratories with **state-of-the-art research equipments**
- ❑ Creation of the chemical library of biologically active compounds, called **the National Library of Biologically Active Compounds (LNCB), unique in Romania**.
- ❑ Achieving the assumed **performance and results' indicators**.

# CURRENT STAGE OF THE PROJECT ACTIVITIES IMPLEMENTATION

## Information and advertising activities

- Project start/end announcement: **1/2**
- Project web-page: **1/1**
- Temporary panel and permanent board: **2/2**
- Participation in project promotion events: **4**
- Project promotion conference: **in progress/1**
- Editing and creating advertising materials (labels, brochures, leaflets, roll-up, *notebooks*, *USB stick*, etc.): **70% / 100%**

- ❑ web page : <https://ro-openscreen.ro/>





# CURRENT STAGE OF THE PROJECT ACTIVITIES IMPLEMENTATION

## Monitoring and reporting activities

➤ *Progress reports and Refund requests:* **12/15**

### Progress of Indicators:

- Projects submitted to EU research programs (no.): **5/3**
- Number of new researchers CO24 (newly created jobs): **1.75/2**
- Number of researchers working in research infr. CO25: **4.73/3**
- New created jobs, other than for researchers (no.): **4/2**
- Number of public-private co-publications: **-/1**
- Nr of equipments: **146(107+39)/146**
- Nr. of necorporals ( licenses and programs): **28/37**
- Newly created/modernized CD laboratories: **in progress/3**
- Modernized area (mp): **in progress/328 mp**

# CURRENT STAGE OF THE PROJECT ACTIVITIES IMPLEMENTATION



- proper insulation
- heat pumps
- heat recovery plant
- photovoltaic panel 90kWh



**C20 and C21 buildings - the final stage of rehabilitation**



# CURRENT STAGE OF THE PROJECT ACTIVITIES IMPLEMENTATION

## Acquisition activities of research equipments and instruments

- ❑ Equipments (pieces): **146**
  - **107** state-of-the-art research equipments and instruments for research
  - **39** IT and communication equipments

***!!! Some of them are unique in Romania***

# Liquid chromatograph/mass spectrometer /diode array

*Unique in Romania*

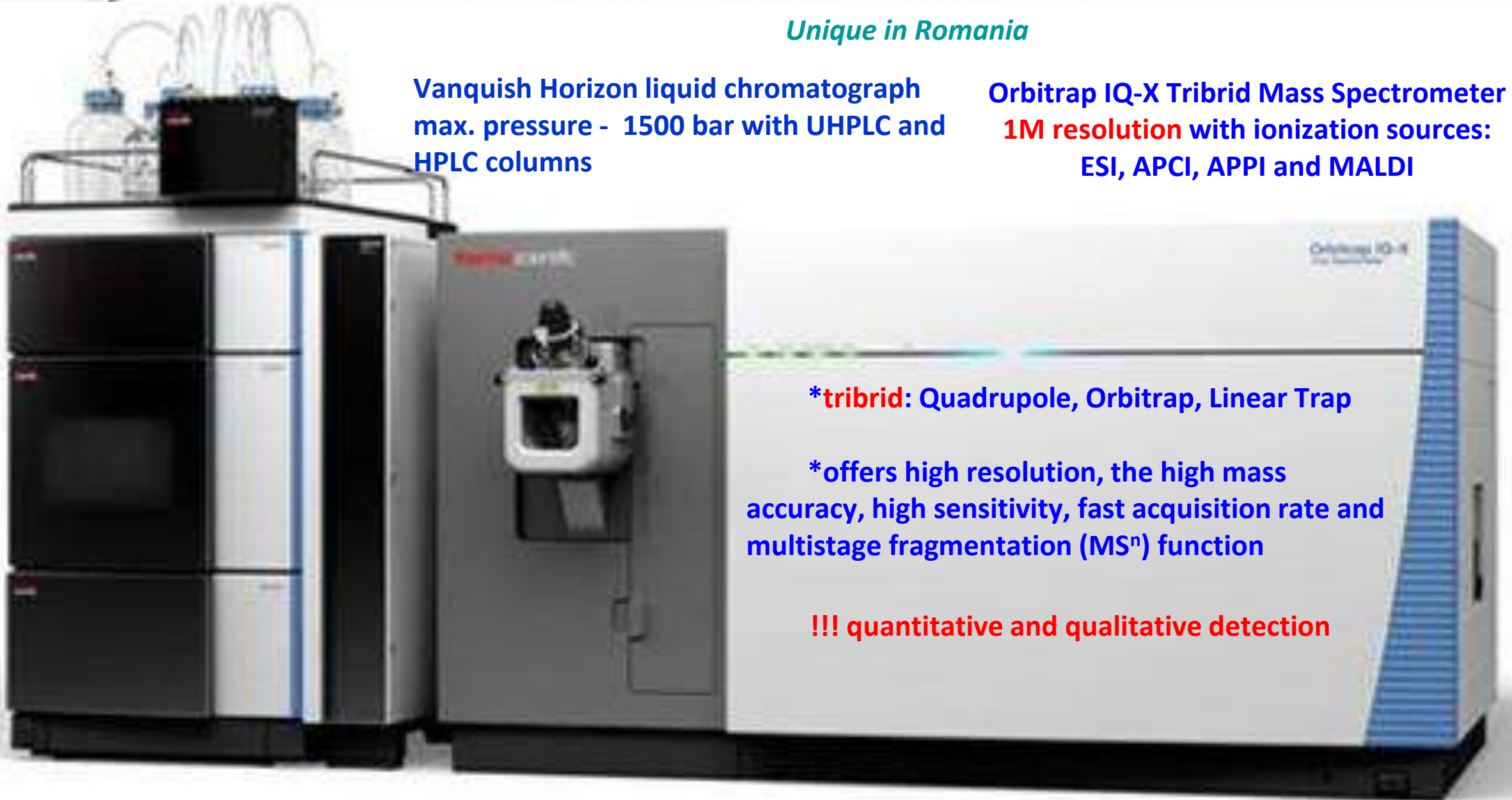
Vanquish Horizon liquid chromatograph  
max. pressure - 1500 bar with UHPLC and  
HPLC columns

Orbitrap IQ-X Tribrid Mass Spectrometer  
**1M resolution** with ionization sources:  
ESI, APCI, APPI and MALDI

\***tribrid**: Quadrupole, Orbitrap, Linear Trap

\*offers high resolution, the high mass  
accuracy, high sensitivity, fast acquisition rate and  
multistage fragmentation (MS<sup>n</sup>) function

**!!! quantitative and qualitative detection**



## Gas Chromatograph/ Mass Spectrometer (GC/MS)



- Agilent 8890GC
- Agilent 7010 triple quad mass spectrometry detector
- Agilent 8697Headspace

**!!! simultaneous qualitative and quantitative detection**

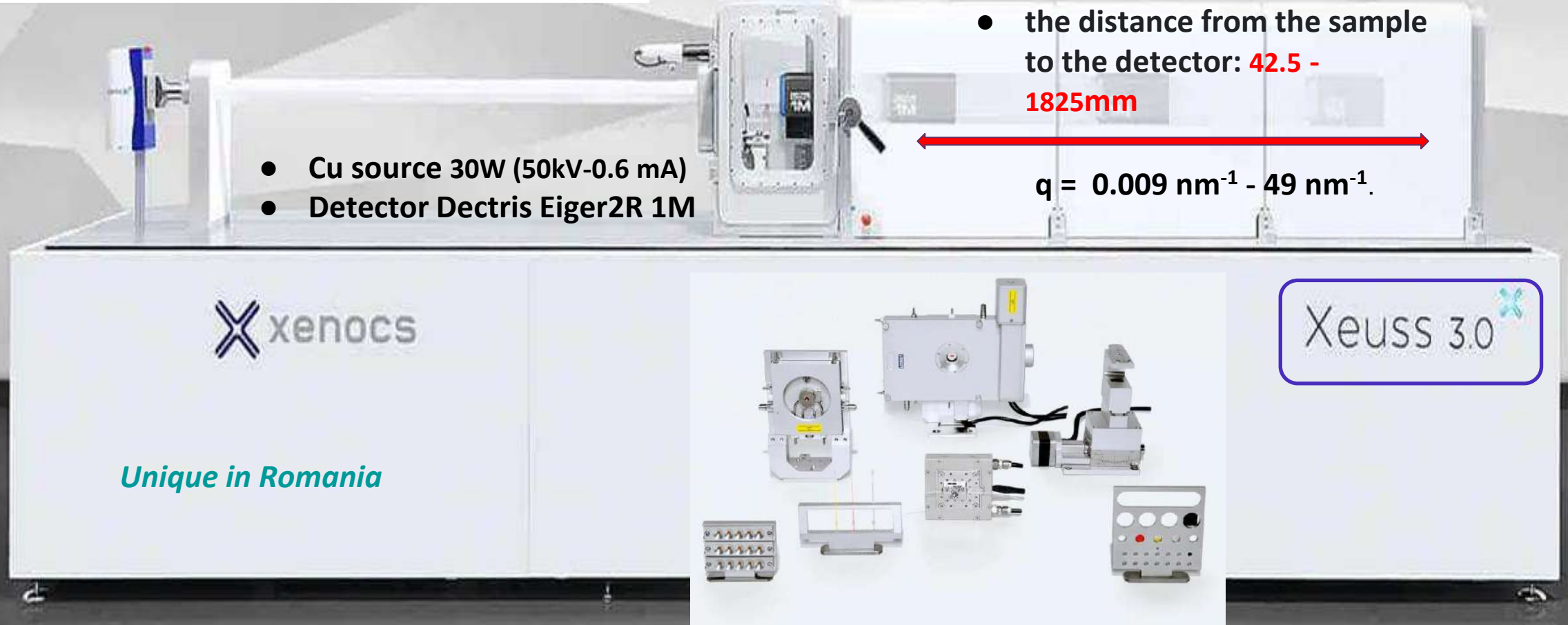
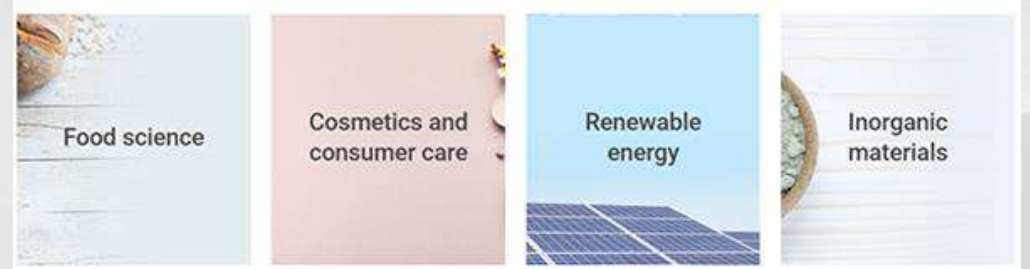
## Elemental Analyzer

Vario EL cube



Detection limit < 50 ppm for C, H, N, S

# SAXS/WAXS diffractometer with GISAXS module



# CIRCULAR DICHROISM/SEMI-PREPARATIVE LIQUID CHROMATOGRAPH

Spectrometer type: Circular Dichroism, J 1500



Integrating sphere with its own detector: JASCO DRCD-575 and JASCO PML-534 detector

Chiroptical spectroscopy has become one of most important techniques for the characterization of biomolecules, determination of absolute configuration and stereochemical analysis

Liquid chromatograph: JASCO LC 4000  
Flux cell: JASCO LCCD-420

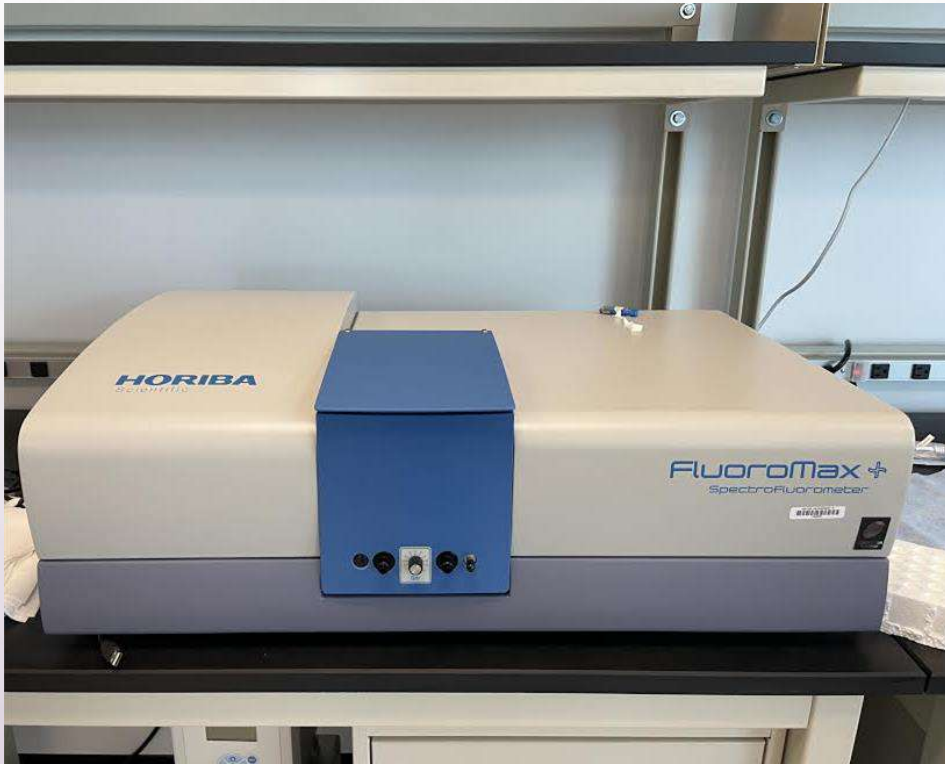
## Accessories:

- Thermostated cell - Linkam 600
- Optical rotatory dispersion (ORD) module: JASCO ORD-520; to measure the chirality of non-absorbing samples and the determination of absolute configuration.



# Spectrofluorimeter and Optical polarizing microscope

**Spectrometer type: FluoroMax+ from HORIBA**



**Sources of excitation: Xe lamp, leds with 370 nm ( $\pm 10$  nm), 470 nm ( $\pm 20$  nm), 635 nm ( $\pm 10$  nm).**

**Carl ZEISS Axiolmager A2m**





## TG/FTIR spectrometer with RAMAN module



- TGA model Discovery TGA 5500, manufacturer TA
- FT-IR model IS-50 with ATR and RAMAN modules, manufacturer Thermo Scientific

# THE NATIONAL LIBRARY OF BIOLOGICALLY ACTIVE COMPOUNDS (LNCB)



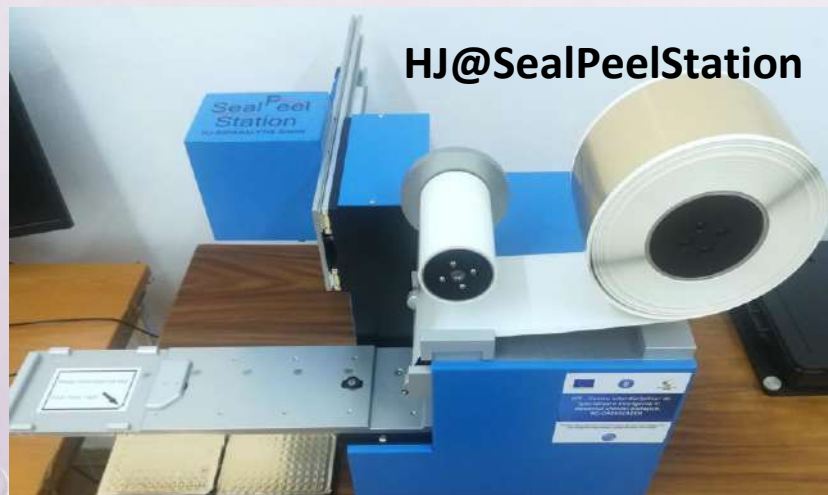
**Automatic workstation -  
Biomek i7 Hybrid (MC +  
Span-8) with Enclosure**



**Echo 650  
Acoustic Liquid  
Handlers**



**Automated Screw Cap  
Decapping**



**HJ@SealPeelStation**

# THE NATIONAL LIBRARY OF BIOLOGICALLY ACTIVE COMPOUNDS (LNCB)

## Thermo Scientific - Varioskan™ LUX multimode microplate reader



## Thermo Scientific - The EVOS M7000 Imaging System



- 2692 approved drugs and natural compounds
- 3000 diversity compounds

were purchased through the project

*compounds selection realized by Ramona Curpan, ICT*

**PĂCUREANU Liliana –  
former project manager**

*Former team members:*

**BANICĂ Cosmin  
DURDUN Mădălina  
MIHAI Corina  
STAN Floare  
STOICA Alina  
URSAN Petru**

*As everyone knows, behind  
every manager is a great and  
very professional **TEAM** and it  
is this whole group that makes  
the*

***RO-OPENSREEN project***

*what it is today!!*

**CSEH Liliana – current project manager**

*The current team members:*

**ANCUȚA Florin  
ANDELESCU Adelina  
BLIDARIU Sergiu  
BORA Alina  
BUTA Ildiko  
CHERA Sofia  
CIOABĂ Sanda  
COSTACHE Ramona  
CRISTEA Diana  
CRIȘAN Luminita**

**CRIȘAN Manuela  
CURPĂN Ramona  
DEVESELEANU Livia  
DRAGOMIR Mirela  
ILIN Alexandru  
POENARU Ana  
STOICA Radu  
STOICHECI Simona  
SUCIU Arleta  
SZERB Elisabeta**

**Big Thanks to all of my colleagues!**

# CONCLUSIONS

## THE RO-OPENSREEN ACHIEVEMENTS:

- ❑ the RO-OPENSREEN Interdisciplinary Center
  - ❑ the high-performance research equipment and tools
    - ❑ the National Library of Biologically Active Compounds (LNCB) (*unique in Romania*)
      - ❑ the high-performance computing system

## TAKE HOME MESSAGE

the main advantage of the facilities through the RO-OPENSREEN interdisciplinary center is the access to high-performance (unique) infrastructure and LNCB resources for all research institutions, universities and the pharmaceutical industry interested to cooperate, on agreed terms.

## COLLABORATION CAN PROMOTE CREATIVITY, INNOVATION AND CROSS-SKILLING!

*even if the projects are finished, the established collaboration remains essential as well as the scientific meetings!*

# THE NATIONAL LIBRARY OF BIOLOGICALLY ACTIVE COMPOUNDS (LNCB)

*unique in Romania*

- the LNCB will be enriched over the next years by a growing number of compounds collected from the Romanian chemistry community, as a wide collaborative effort toward the common objective of building a best-in-class library to accelerate the drug discovery process, and beyond



## Compound Management Facility

- Compound registration & reformatting
- Bioprofiling Assays: Solubility, ROS (Reactive Oxygen Species)

Library copies



## Screening Partner Site

Institute of Biochemistry of the Romanian Academy, Bucharest



**Your compounds are welcome in our LNCB !**



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**THANK YOU FOR YOUR ATTENTION!**

