

# Nuclear Magnetic Resonance and Mass Spectrometry Laboratory

University of Rome "Tor Vergata"

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Department of Chemical Sciences  
and Technologies





# The lab





## Nuclear magnetic resonance (NMR)

is a very powerful analytical technique used to study different types of compounds such as small molecules (active pharmaceutical ingredients or metabolites), natural products, polymers, biomolecules (proteins, nucleic acids, carbohydrates, lipids) and other. In fact, by measuring the absorption of electromagnetic radiation in molecules immersed in a strong magnetic field, it is possible to obtain detailed information either on the molecular structure of the compounds under examination or the composition of a complex mixture. Its applications concern the determination of the three-dimensional structure of a pharmacological target, the characterization of possible drugs, and their interaction with targets through in vitro dynamics studies, or possibly through the metabolic response that drug administration can produce in a animal and / or human organism. It is in this last field that the NMR sees its innovative application, it is in fact possible to observe and rigorously quantify all the most abundant components present in biological fluids such as urine, blood, saliva, cell extracts and tissues, without the need of long and elaborate preparations.





## UHPLC- Accurate-Mass Q-TOF (UHPLC-HRMS)

High-performance liquid chromatography (HPLC) is a very powerful separation method widely used in environmental science, pharmaceutical industry, biological and chemical research and other fields. Generally, it can be used to purify, identify and/or quantify one or several components in a mixture simultaneously.

Mass spectrometry (MS) is a detection technique by measuring mass-to-charge ratio of ionic species. The procedure consists of different steps. First, a sample is injected in the instrument and then evaporated. Second, species in the sample are charged by certain ionized methods. Finally, the ionic species will be analyzed depending on their mass-to-charge ratio ( $m/z$ ) in the analyzer.

The mass spectrometric identification is widely used together with chromatographic separation. Our instrument uses electrospray ionization (ESI) for the generation of the ions and the Q-TOF analyzer which gives accurate mass measurements, coupled with an UHPLC system.

The LC has an efficient capacity of separation and MS has a high sensitivity and strong ability of structural characterization. Furthermore, TOF-MS, has several distinctive properties on top of regular MS, including fast acquisition rates, high accuracy in mass measurements and a large mass range. The combination of LC and ESI-TOF-MS allow us to obtain a powerful tool in the quantitative and qualitative analysis of molecules in complex matrices by reducing the matrix interferences.





# The research



# What we can do

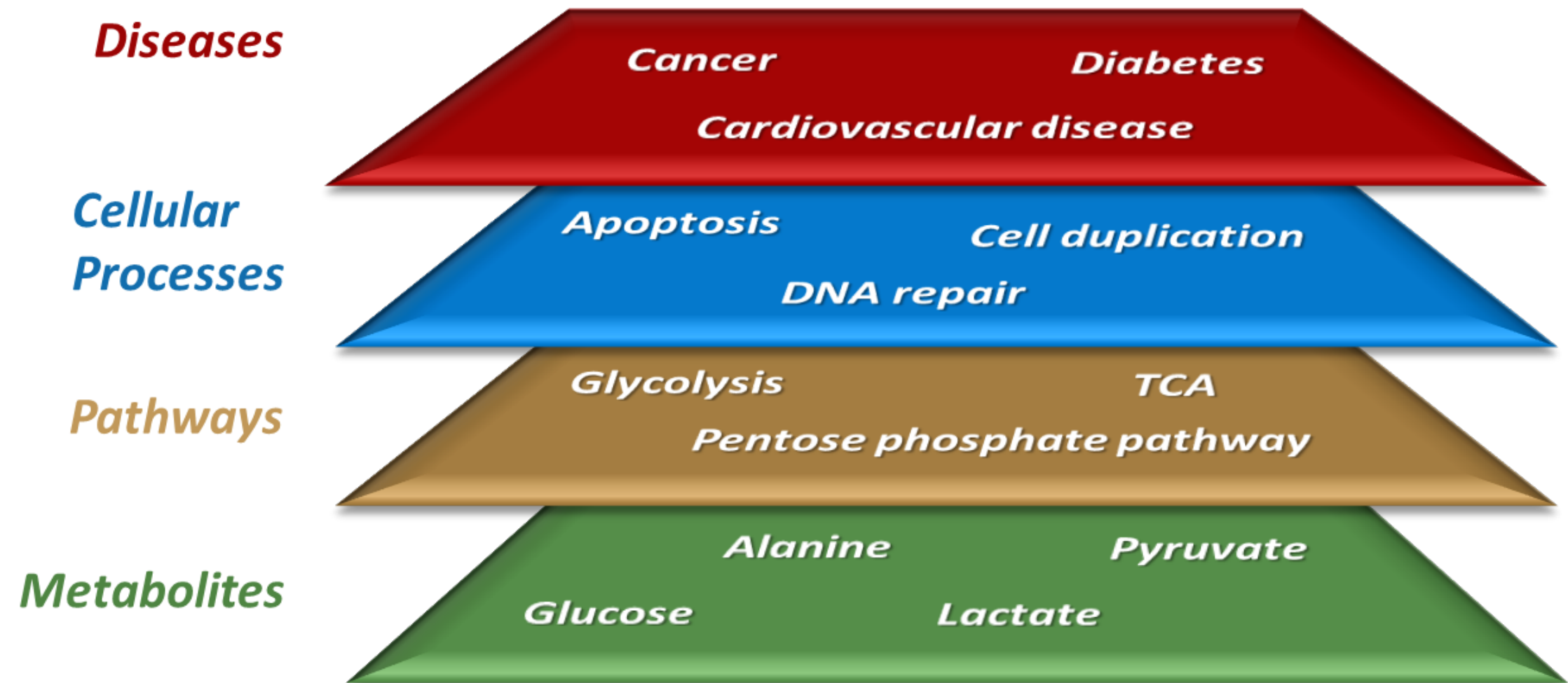
- Structural check, purity and stability
- Analysis of the aggregation status
- Determination of the three-dimensional structure of macromolecules
- Protein / ligand interaction studies
- Metabolomics studies



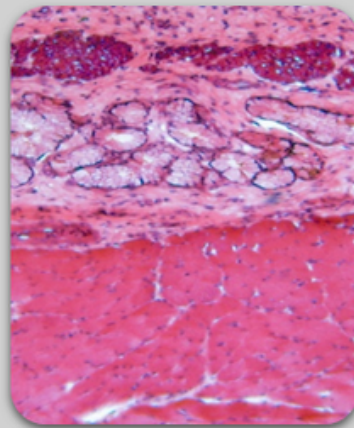
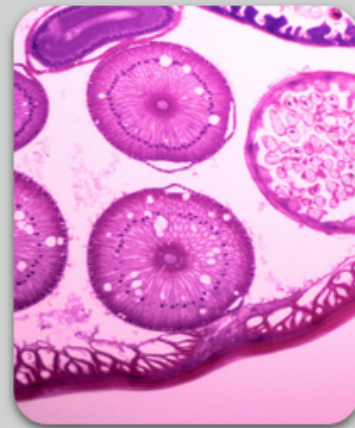
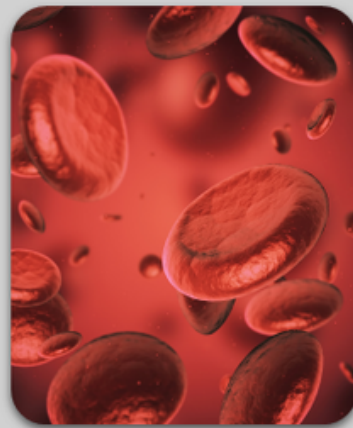


Among the omic sciences such as transcriptomics, proteomics and genomics, the one that refers to the study of small molecules (MW <1500Da) is called Metabolomics. The possibility of observing how the concentrations of metabolites (lactate, glucose, pyruvate, amino acids, ...) vary according to pathophysiological stimuli, represents a great potential in the search for biomarkers of diseases, and in their contextualization within biochemical pathways. However, this scientific approach is not only limited to a clinical setting, but can be expanded for all its potential to the observation of any biophysical question, from the agri-food sector to that of biomaterials.

# Metabolomics



# Types of samples used in our metabolomics studies



**Biofluids:**  
Plasma,  
Urine,  
Saliva,  
CSF,  
...

**Cell,  
micro-  
organism  
or  
bacterium  
extracts**

**Cell,  
micro-  
organism  
or  
bacterium  
culture  
media**

**Tissue:**  
Muscle,  
Bone  
marrow

**Plant  
extracts**

**Food:**  
Meat,  
cheese,  
vegetable,  
oil, wine,  
beer,...

**Other  
complex  
mixtures:**  
Soil,  
Marine  
sediments,  
River and  
sea  
waters,...



# Some of our publications

Structure 14, 309–319, February 2006 ©2006 Elsevier Ltd All rights reserved DOI 10.1016/j.str.2005.11.012

## Molecular Basis for Phosphorylation-Dependent, PEST-Mediated Protein Turnover

J. Am. Chem. Soc. 1995, 117, 1027–1033

1027

Maria M. García-Alai,<sup>1,4</sup> Mariana Gallo,<sup>2,4</sup>  
Marcelo Salame,<sup>1</sup> Diana E. Wetzler,<sup>1</sup>  
Alison A. McBride,<sup>3</sup> Maurizio Paci,<sup>2</sup> Daniel O. Cicero,<sup>2</sup>  
and Gonzalo de Prat-Gay<sup>1,\*</sup>

NMR Analysis of Molecular Flexibility in Solution: A New Method for the Study of Complex Distributions of Rapidly Exchanging Conformations. Application to a 13-Residue Peptide with an 8-Residue Loop

D. O. Cicero, G. Barbato, and R. Bazzo\*

Contribution from the Istituto di Ricerche di Biologia Molecolare (IRBM) P. Angeletti, via Pontina km 30,600, (00040) Pomezia, Rome, Italy

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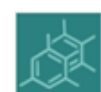
Virology

journal homepage: [www.elsevier.com/locate/yviro](http://www.elsevier.com/locate/yviro)



Structural characterization of the Hepatitis C Virus NS3 protease from genotype 3a: The basis of the genotype 1b vs. 3a inhibitor potency shift

Mariana Gallo<sup>a,1</sup>, Matthew James Bottomley<sup>b,1</sup>, Matteo Pennestri<sup>a</sup>, Tommaso Eliseo<sup>a</sup>, Maurizio Paci<sup>a</sup>, Uwe Koch<sup>b</sup>, Renzo Bazzo<sup>a,b</sup>, Vincenzo Summa<sup>b</sup>, Andrea Carfi<sup>b</sup>, Daniel O. Cicero<sup>a,\*</sup>



molecules



Article

## Personalized Metabolic Profile by Synergic Use of NMR and HRMS

Greta Petrella<sup>1</sup>, Camilla Montesano<sup>2</sup>, Sara Lentini<sup>1</sup>, Giorgia Ciufolini<sup>1</sup>, Domitilla Vanni<sup>1</sup>, Roberto Speziale<sup>3</sup>, Andrea Salonia<sup>4,5</sup>, Francesco Montorsi<sup>4,5</sup>, Vincenzo Summa<sup>3</sup>, Riccardo Vago<sup>4,5</sup>, Laura Orsatti<sup>3</sup>, Edith Monteagudo<sup>3</sup> and Daniel Oscar Cicero<sup>1,\*</sup>

## PLOS NEGLECTED TROPICAL DISEASES

OPEN ACCESS PEER-REVIEWED

RESEARCH ARTICLE

## Drug effects on metabolic profiles of *Schistosoma mansoni* adult male parasites detected by <sup>1</sup>H-NMR spectroscopy

Alessandra Guidi, Greta Petrella, Valentina Fustaino, Fulvio Saccoccia, Sara Lentini, Roberto Gimmelli, Giulia Di Pietro, Alberto Bresciani, Daniel Oscar Cicero, Giovina Ruberti



metabolites



Article

## Metabolic Reprogramming of Castration-Resistant Prostate Cancer Cells as a Response to Chemotherapy

Greta Petrella<sup>1,\*</sup>, Francesca Corsi<sup>2,†</sup>, Giorgia Ciufolini<sup>1</sup>, Sveva Germini<sup>1</sup>, Francesco Capradossi<sup>2</sup>, Andrea Pelliccia<sup>1,2</sup>, Francesco Torino<sup>3</sup>, Lina Ghibelli<sup>2,†</sup> and Daniel Oscar Cicero<sup>1,†</sup>



International Journal of  
Molecular Sciences



Article

## The Interplay between Oxidative Phosphorylation and Glycolysis as a Potential Marker of Bladder Cancer Progression

Greta Petrella<sup>1</sup>, Giorgia Ciufolini<sup>1</sup>, Riccardo Vago<sup>2,3,\*</sup> and Daniel Oscar Cicero<sup>1,\*</sup>



# Reach out

## Scientific direction

Prof. Daniel Oscar Cicero

## Research fellow

Dr. Greta Petrella

## Technical assistance

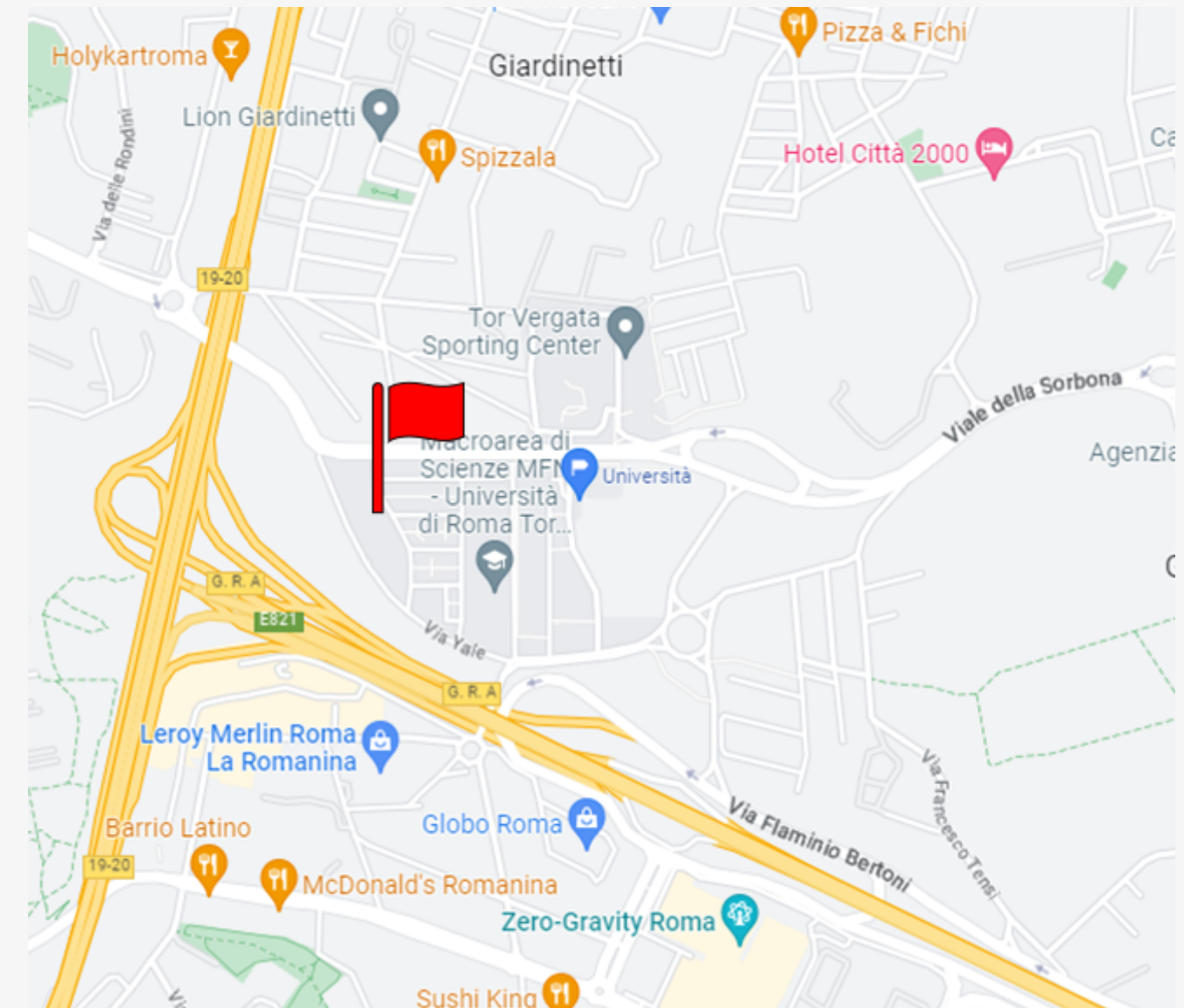
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