

# *High resolution 600 MHz NMR spectrometer equipped with cryo-probe*

**Project title: High resolution NMR spectroscopy -  
from molecular structure to foods, nutrition and human health**

**Proponente: prof. Alfredo Miccheli**

**Co-proponenti: prof. Lorenzo Maria Donini, prof. Federico Marini**



**SAPIENZA**  
UNIVERSITÀ DI ROMA

**«Presentazione alla  
Comunità Sapienza delle Grandi  
Attrezzature di Ateneo»  
13 maggio 2019, Aula Magna del Rettorato**

# *High resolution 600 MHz NMR spectrometer equipped with cryo-probe*

- The NMR instrument should be a JEOL ECZR serie (provisional adjudication) equipped with a 5 mm probe for  $^1\text{H}$ ,  $^{19}\text{F}$ ,  $^{13}\text{C}$  and from  $^{31}\text{P}$  to  $^{15}\text{N}$  experiments and a cryo-probe supercool for  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$ ,  $^{15}\text{N}$  experiments. All omo- and heteronuclear bidimensional experiments are guaranteed. The cryo-probe increases the sensitivity of  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$  by 2-3 folds.
- This instrument allows to identify the structure of molecules in solution and to quali-quantitatively determinate low molecular weight compounds in natural mixtures (such as liquid samples originated from microbes, foods, plant and animal cells, tissues and organs, human and animal biological fluids).

## High resolution 600 MHz NMR spectrometer equipped with cryo-probe



**A cooled autosampler for 30 tubes  
will be provisionally provided on  
approval**

- **13 Departments**
- **4 Faculties:**
- **SFMN, Pharmacia and Medicine,  
Medicine and Dentistry, Civil  
and Industrial Engineering.**
- **44 subscribers**
- **The instrument will be  
installed in the Department  
of Chemistry, CU014  
building, room 059, ground  
floor. The complete  
installation is expected for  
the end of October.**

# High resolution 600 MHz NMR spectrometer equipped with cryo-probe

**Chemical Structure**  
25% of total activity



**Metabolomics**  
75% of total activity

**NMR-based Metabolomics Laboratory of  
Sapienza**

# Organization and regulations for the utilization of the NMR-based Metabolomics Laboratory of Sapienza

## Scientific coordination:

- The committee has been selected among the co-proponents or signatory proponents of the project GA (2016) and supervised by prof. **Alfredo Miccheli** (proponent). The committee is composed by 6 members of Departments which have expressed a larger number of research lines in Metabolomics.
- The six members of Departments are:
  - Biology and Biotechnology "Charles Darwin" (prof. **D. Uccelletti**)
  - Chemistry (prof. **Federico Marini**)
  - Chemistry and Technology of Drugs (prof. **L. Mannina**)
  - Environmental Biology (prof. **G. Pasqua**)
  - Experimental Medicine (prof. **L.M. Donini**)
  - Physiology and Pharmacology "Vittorio Erspamer" (prof. **C. Limatola**)

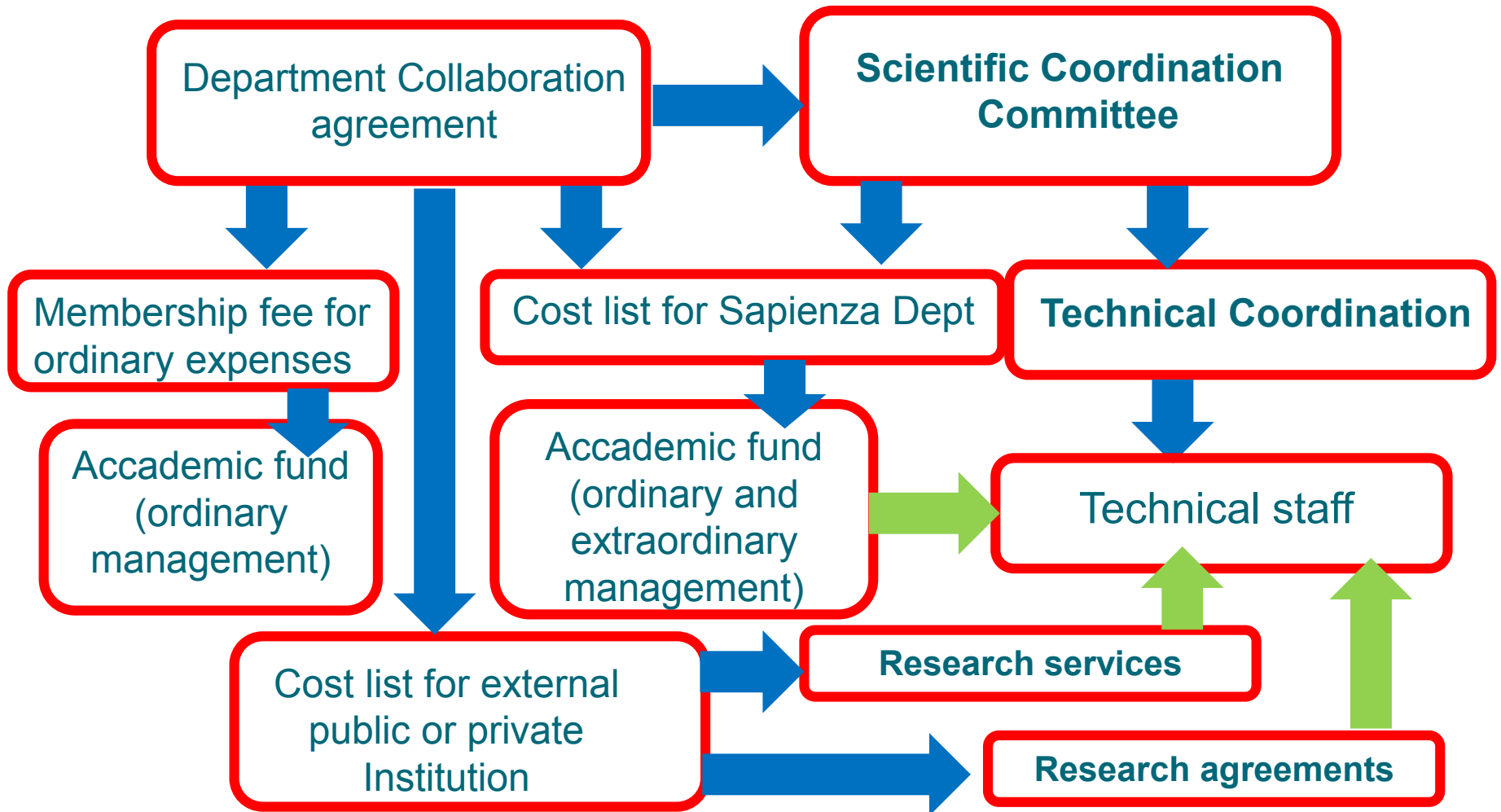
## Technical coordination:

dr. **Giorgio Capuani** (Department of Chemistry)

## Organization and regulations to utilize the NMR-based Metabolomics Laboratory of Sapienza

1. The 6 Departments are proceeding to formulate a **Collaboration Agreement (to be confirmed in the respective Councils)** that provides for an annual membership fee of 5.000 Euro for each Department, in order to cover the annual ordinary expenses of the Laboratory. Therefore, a fund (project) for this management purpose shall be opened by the Chemistry Department, where the instrument will be allocated. (This solution simplifies the procedure for the supply cost of cryogenic gas, N<sub>2</sub> gas and for the He refilling service). In this fund (project) also the budgets from the other Departments of Sapienza will merge, as defined by the price list. External services will merge in suitable funds of either the Department of Chemistry or the other Departments depending on the specific agreement.
2. The **Collaboration Agreement** among the 6 Departments defines the available machine-time (60% of the time is devoted to researches and collaborations of the 6 Departments and the remaining 40% is devoted to researches requested by other Sapienza Departments or by external public or private institutions); updates the cost list; regulates the access of the staff authorized to use the instrumentation.

# Organization of the NMR-based Metabolomics Laboratory of Sapienza



## Research service by NMR-based Metabolomics Laboratory

1. Sample conservation at  $-80^{\circ}$  C until analysis.
2. Sample preparations with deuterated solvents and standard references.
3. NMR tubes supply;
4.  $^1\text{H}$  NMR monodimensional spectra acquisition by NMR quantitative procedure;
5. ( $^1\text{H}$ - $^1\text{H}$  e  $^1\text{H}$ - $^{13}\text{C}$ ) NMR bi-dimensional spectra acquisition to assign the compounds;
6. Spectral processing, assignment and integration of the resonances;
7. Results of qualitative and quantitative analysis reported in excel format.



# Cost list

## External research service

- Standard monodimensional  $^1\text{H}$  NMR: 80 euro; 130 euro with cryoprobe.
- $^{13}\text{C}$ ,  $^{31}\text{P}$ ,  $^{19}\text{F}$ ,  $^2\text{H}$  NMR monodimensional experiments: 200 euro; 250 euro with cryoprobe.
- Omo-nuclear o hetero-nuclear bidimensional spectrum: 400 euro.
- Sample preparation (steps 2 and 3) an additional cost of 30 euro for each sample.

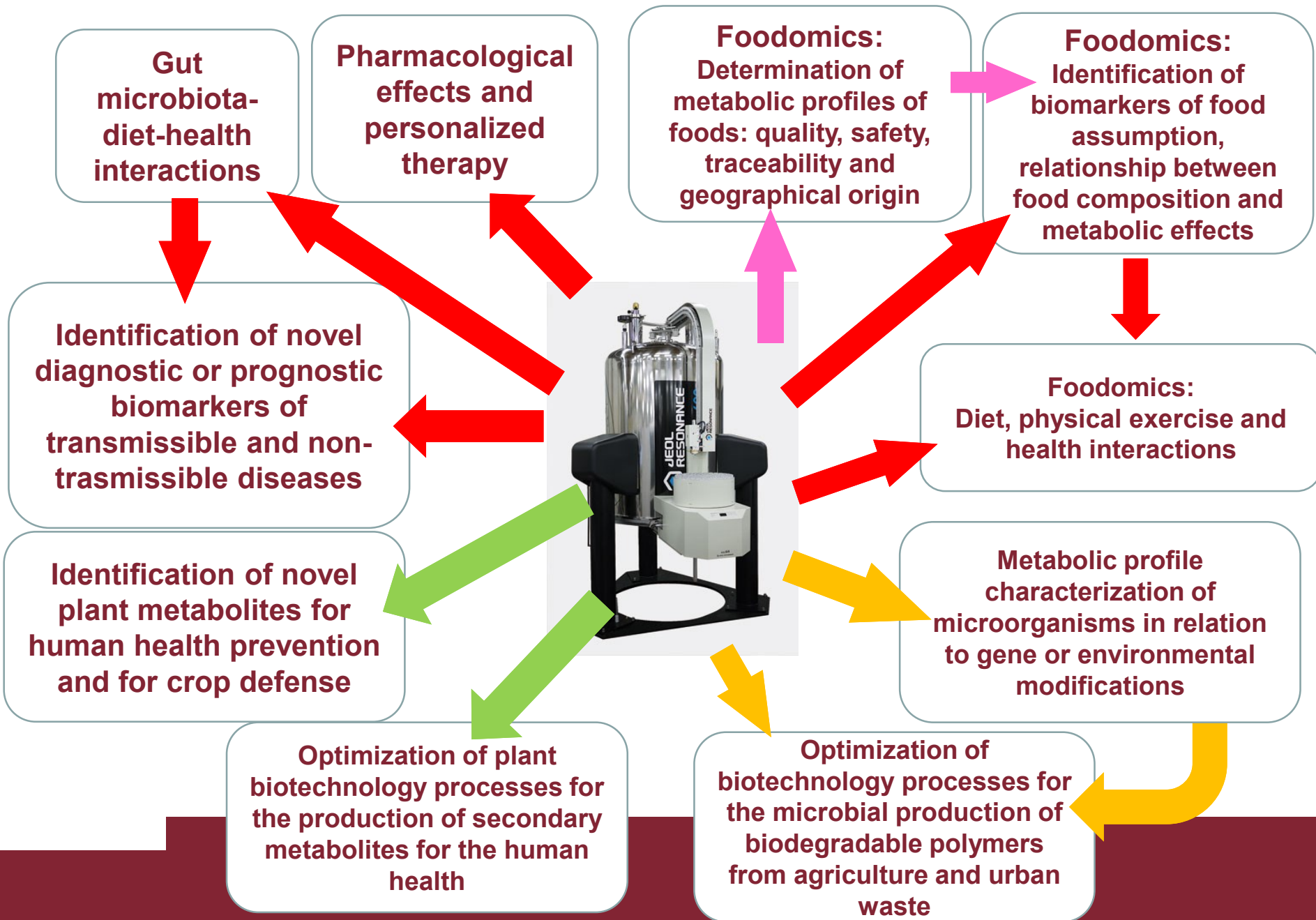
## Research Service for Sapienza

- 50% less than the external cost list

## Member Department of the Management Committee.

- Each Member has 3 days/month of machine-time

# Ongoing or planned Research Lines



# Accademic research projects in progress - 2019

1. Sustainable cultivation of the medicinal plant *Hypericum perforatum* (L.): soil saprotrophic fungi for growth promoting and resistance-induction.

(progetto di Ricerca Ateneo 2018. Department of Environmental Biology) Principal Investigator: **Prof.ssa A. M. Persiani**; Funds **Euro 31.000 + 23.800** (research grant).

2. Study of Metagenomic and Metabolomic Profiles of Gut Microbiota and Intestinal Immunological Network in Children with Crohn's Disease treated with Partial Enteral Nutrition as a Strategy for maintaining disease remission. (progetto di Ricerca Ateneo 2018, Department of Pediatrics and Child Neuropsychiatry). Principal Investigator: **Prof. S. Cucchiara**; Funds **Euro 25.000**.

3. Identification and Characterization of novel epigenetic factors and metabolic control. (progetto di Ricerca Ateneo 2018, Department of Biology and Biotechnologies, C. Darwin). Principal Investigator: **Prof. G. Camilloni**; Funds Euro **12.500**.

## Research projects in progress 2019-2020

- “*Strategie innovative per un latte di qualità*” (StraLaQ). PROGETTI MIPAFPT "FONDO LATTE D.M. n. 27443 DEL 25/09/2018. Responsabile prof **Stefano Materazzi**. Dipartimento di Chimica Sapienza - Dipartimento di Medicina Veterinaria UNIMI. Euro 281.579 (**Sapienza Euro 164.759**)
- Contratto di ricerca con Azienda Agricola M. Aureli all'interno degli obiettivi realizzativi del progetto **Innovazione sostenibile per le produzioni agroalimentari di qualità - INNOPAQ**: nell'ambito dei progetti POR FESR Abruzzo 2014-2020 : Linee di azione **1.1.1 e 1.1.4**. Titolo del progetto di ricerca: “Applicazione di tecniche innovative analitiche per la ottimizzazione delle fasi del processo: raccolta, trasformazione e conservazione di prodotti vegetali”. Responsabile prof. **Alfredo Miccheli. Euro 65.000**
- Contratto di Ricerca con Azienda Agricola M. Aureli “Sviluppo di nuovi alimenti vegetali funzionali al benessere della salute e di nuovi processi di sanificazione di alimenti ”. Responsabile prof. **Alfredo Miccheli. Euro 39.000**

# Public Institutions that have expressed potential interest to NMR-based Metabolomics Laboratory Service

- Direzione Scientifica Ospedale Pediatrico Bambino Gesù (Metabolomics of gut microbiota)
- INAIL (occupational medicine: predictive metabolic biomarkers of injury).

# Provisional Contacts

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Web site in progress



## Ringraziamenti

- I RAD: dott.ssa Lisena Rubini, Giovanna Bianco e Angela Chiaranza per avermi sopportato e supportato nella stesura dell'accordo di collaborazione tra Dipartimenti;
- La dott.ssa Francesca Cosi e il personale del Settore Gare forniture e servizi per avermi messo in condizione di comprendere le procedure per le Gare.
- Il RUP dott. Giorgio Capuani e il RAD dott.ssa Giovanna Bianco per la loro pazienza e abilità a districarsi nei meandri delle procedure.