Finanziato dall'Unione europea NextGenerationEU | Ministero dell'Università e della Ricerca | Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA | Consiglio Nazionale delle Ricerche

ITACA·SB

Potentiating the Italian Capacity for Structural Biology Services in Instruct-ERIC

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Annex I – CNR Service catalogue

Transnational Access (TNA) @ National Research Council

version 1.2 – December 12th, 2025
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version 1.0 – February 15th, 2025

CNR | Istituto di Cristallografia - Via Giovanni Amendola, 122/O - 70126 Bari (ITALIA)
Direzione +39 080 5929167
Segreteria/Amministrazione +39 080 5929142 / +39 080 5929141
E-mail: segreteria@ic.cnr.it - **Sito web:** www.ic.cnr.it
P.IVA 02118311006 - C.F. 80054330586

The analysis and services provided by the ITACA.SB research infrastructure are carried out across multiple CNR Operative Units (O.U.), each equipped with specialized resources and expertise to support a diverse range of experimental and/or computational activities.

The complete list of services is provided below, categorized by O.U.:

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Operative Unit CNR-IC Bari

Institution
CNR, Istituto di Cristallografia (IC)
Via Giovanni Amendola 122/O - 70126 Bari
Website: https://www.ic.cnr.it

ITACA.SB service coordinator at the O.U.: Dr. Cinzia Giannini

Services list at CNR-IC Bari:

HPC

- **Service ID**: BAHP
- **Name**: High Performance Computing Cluster
- **Description**: High Performance Computing cluster designed to provide support to the scientific community for CryoEM, BioSAXS, X-Ray data storage and processing, as well as to enhance theoretical and computational research in Structural Biology and Drug Discovery
- **Equipment**:
  - 5x compute nodes Dell PowerEdge R760 (2x Intel Xeon Gold 6448Y 2.1G, 32C/64T, 16GT/s, 60M Cache; 1024GB RAM 4800MHz DDR5);
  - 4x GPU nodes Dell PowerEdge R760XA (4x GPU Nvidia H100 94GB NVLINK Bridge);
  - 2x Login/service nodes Dell PowerEdge R760xs;
  - Storage Scale-Out NAS 4x Dell PowerScale Isilon A3000 nodes (1280 TB raw space);
  - Schrödinger Suite including Docking and Virtual Screening, Molecular Dynamics Simulation, Homology Modelling, and QSAR and cheminformatics models
  - Computational Chemistry software including CP2K, Nwchen, DeepMD
  - Gromacs, NAMD, LAMMPS for Molecular Dynamics and Structural Biology solutions
- **Cost**:
  - CPU core - € 0,007/hour
  - CPU node (64 cores) - € 10,75/day
  - GPU - € 0,21/hour
  - GPU node (4 GPU) - € 20,16/day

BioSAXS

- **Service ID**: BASX
- **Name**: Small Angle X-Ray Scattering analysis on biological macromolecules in solution

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- **Description**: characterization of biological specimen under native-like conditions to assess oligomeric states and conformational changes as a function of time, pH, ionic strength, and temperature:
  - WAXS - Wide Angle X-ray Scattering;
  - SAXS - Small Angle X-ray Scattering;
  - GIWAXS - Grazing Incidence Wide Angle X-ray Scattering;
  - GISAXS - Grazing Incidence Small Angle X-ray Scattering;
  - USAXS - Ultra Small Angle X-ray Scattering;
  - SAXS Scanning Microscopy;
  - WAXS Scanning Microscopy;
  - SEC-SAXS Size Exclusion Small Angle X-ray Scattering;
  - SWAXS Contemporary SAXS and WAXS data collection;
  - Peltier in Transmission Geometry;
  - Peltier in Reflection Geometry;
  - Shear Cell;
  - Reactivity Chamber;
- **Equipment**:
  - XEUSS3.0 system (HR model) equipped with a motorized dual source: Ga Excillum liquid jet source and Cu micro-source;
  - Detector: Eiger 2R (1M), moving in vacuum from 42.5 mm to 1800 mm (sample-to-detector distance);
  - Bonse-Hart 4-bounce Si(111) channel cut crystals monochromator and analyzer for uSAXS;
  - Biocube system. Size-exclusion chromatography is coupled with SAXS (SEC-SAXS) using an AKTA go™ protein purification system;
  - 4-Axis motorized SWAXS module with EIGER2 R 500K: covering 1/8th of Ewald sphere in forward scattering. Achieved 2Theta range for scattering is from 7° to 90°. Rotation travel in perpendicular plane is 90° for in plane scattering or collection at high azimuth angles. Includes vertical translation to move the detector out of the chamber and control of detector inclination;
  - Low Noise Flow Cell: Vacuum compatible low scattering flow cell for measurements on liquids. Manual injection with large volume as well as with volumes down to a few µL with a no dead volume solution from syringe to the cell;
  - Xenocs Couette stage for shear SAXS: In air operated coaxial cylindric shear stage with external cylinder rotor (Couette type) and temperature control of stator. 1mm fixed gap between stator and internal surface of rotor. Rotational and oscillatory modes;
  - Advanced GISAXS module for thin films including Omega, Ry and Psi rotations;

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  - Multisample holder for powders and gels (also suitable for liquids);
  - Multi-purpose X-Ray Temperature Stage (-20 to 150°C): Peltier type temperature stage for heating and cooling adapted for solids, gels, powders and capillaries. Compatible with GISAXS and Xenocs low noise flow cell Temperature range reduced to 4°C to 50°C for liquid samples.
- **Cost**: € 60/hour

BioSAXS data analysis (Offline)

- **Service ID**: BSDA
- **Name**: BioSAXS data analysis
- **Description**: extensive analysis of BioSAXS data collected either at the BioSAXS ITACA.SB Operative Unit in Bari or elsewhere.
- **Equipment**:
  - SAXS software package developed in-house
- **Cost**: € 43/hour

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Operative Unit CNR-IC URT Caserta

Institution
CNR, Istituto di Cristallografia (IC) URT Caserta
c/o Dipartimento di Scienze e Tecnologie Ambientali, Biologiche e Farmaceutiche (DiSTABiF) Università degli Studi della Campania "Luigi Vanvitelli", Via Vivaldi 43 - 81100 Caserta
Website: https://www.ic.cnr.it/sede/caserta

ITACA.SB service coordinator at the O.U.: Dr. Michele Saviano

Services list at CNR-IC URT Caserta:

Protein production

- **Service ID**: CEPP
- **Name**: large scale protein expression (recombinant in *E. coli*) and purification
- **Description**: expression and purification of proteins using bacterial cells as a host system
- **Equipment**:
  - vertical autoclave (T-Lab Eco V60)
  - 2x shaking incubators (SKI 8 R)
  - 2x standard Beckman centrifuges: (Avanti J26S XP and Allegra V-15R) equipped with different sets of rotors.
  - sonicator (Vibra-Cell™ VCX 130)
  - UV/Vis spectrophotometer for nano volume and cuvette (Implen NanoPhotometer™ NP80)
  - ÄKTA pure 25M FPLC System
  - Dynamic Light Scattering (Zetasizer Pro Blue)
- **Cost**: € 4.500,00/sample

CryoEM

- **Service ID**: CEEM
- **Name**: CryoEM sample preparation and data collection
- **Description**: comprehensive characterization of vitreous biological specimens, encompassing sample vitrification, screening, and data collection.
- **Equipment**:
  - TFS 200 kV Transmission Electron Cryo-Microscope (Glacios 1™)
  - Vitrobot Mark IV™
- **Cost**: € 1.094,56/day

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CryoEM - Data Analysis

- **Service ID**: CEDA
- **Name**: CryoEM data analysis
- **Description**: Single Particle Analysis (SPA) of cryoEM data (up to electron density map)
- **Equipment**:
  - 2x compute node (each with 4x NVIDIA RTX A5000 Graphics Cards, 24GB GDDR6X, 2x Intel Xeon Scalable Silver 4314 Processor 16-Core 2.4GHz)
  - 1x compute node (8x NVIDIA RTX A5000 Graphics Cards, 24GB GDDR6X, 2x Intel Xeon Scalable Gold 5320 Processor 26-Core 2.2GHz)
  - Storage node (~500 TB of raw storage for temporary data storage)
- **Cost**: € 800 (using Relion 5.0)

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Operative Unit CNR-ICB Catania

Institution
CNR, Istituto di Chimica Biomolecolare (ICB) sede secondaria di Catania
Via Paolo Gaifami, 18 – 95126 Catania
Website: https://www.icb.cnr.it/icb-home-it/sede-secondaria-di-catania

ITACA.SB services coordinator at the O.U.: Dr. Nicola D'Antona

Services list at CNR-ICB Catania:

Mass Spectrometry

- **Service ID**: CTMS
- **Name**: Matrix-Assisted Laser Desorption/Ionization-Time of Flight (MALDI-TOF) structural analysis
- **Description**: identify and separate a wide variety of compounds ranging from chemical to biological entities, based on their mass-to-charge ratio (m/z):
  - Intact protein characterization for determining the molecular weight, structure, and post-translational modifications (Linear mode - up to 600 kDa)
  - Peptide characterization from in-gel digestions (Reflector mode)
  - Analysis of Polysaccharides (oligo/complex carbohydrates) (Reflector mode)
  - Glycoproteins and Glycopeptides: glycan profiling (Reflector mode)
  - Polymer analysis (Reflector mode)
  - MS/MS analysis for Peptide and Protein Identification
  - MS/MS analysis for Small Molecule Identification
  - MS/MS analysis for Quantification of Targeted Compounds
  - MS/MS analysis for Analysis of Post-Translational Modifications
  - MS/MS analysis for Structure Elucidation
  - MS/MS analysis for Metabolomics
- **Equipment**:
  - UltrafleXtreme MALDI-TOF/TOF with 5 GS/s 10 bit digitizer for enhanced resolution and dynamic range
- **Cost**: € 200,00/sample/hour

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Operative Unit CNR-IBPM Rome

Institution
CNR, Istituto di Biologia e Patologia Molecolari (IBPM)
c/o Dipartimento di Scienze Biochimiche "Alessandro Rossi Fanelli"
Sapienza Università di Roma, Piazzale Aldo Moro 5 – 00185 Roma
Website: https://www.ibpm.cnr.it

ITACA.SB service coordinator at the O.U.: Dr. Andrea Ilari

Services list at CNR-IBPM Rome:

High-Throughput Crystallization

- **Service ID**: RMHT
- **Name**: High-throughput crystallization of soluble and membrane proteins
- **Description**: Screening of crystallization conditions to produce highly diffracting crystals of proteins amenable to X-ray crystallography (structure determination)
- **Equipment**:
  - Oryx8 high throughput crystallization robot (Douglas Instruments)
  - SteREO Discovery V20 KMAT stereomicroscopes equipped with an AXIOCAM full 4K camera (Zeiss), XtalLight X100 fluorescence instrument (XtalConcepts)
  - Nanodrop One (Thermofisher Scientific)
- **Cost**: € 755,79 (includes: 4x 96-well plates, 4x Axygen deepwell 2.0 mL (50 pcs), 4x Aluminum Sealing Film)

Crystal optimization

- **Service ID**: RMCO
- **Name**: Optimization of crystallization conditions based on 2D gradients, cross-matrix optimization, additive scatter optimization and matrix microseeding
- **Description**: visual inspections of crystallization plates
- **Equipment**:
  - Oryx8 high throughput crystallization robot (Douglas Instruments)
  - SteREO Discovery V20 KMAT stereomicroscopes equipped with an AXIOCAM full 4K camera (Zeiss), XtalLight X100 fluorescence instrument (XtalConcepts)
  - Nanodrop One (Thermofisher Scientific)
- **Cost**: see High-throughput crystallization (combined service)

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Surface Plasmon Resonance

- **Service ID**: RMSP
- **Name**: Determination of binding constants for protein-protein and protein-small ligands (>200 Da) interactions
- **Description**: High-throughput surface plasmon resonance for faster hit identification. Two standard injection formats: OneStep® Injection Technology and industry standard multi-cycle kinetics (MCK). Binding sensorgrams are analysed using the SARTORIUS built-in analysis software
- **Equipment**:
  - Octet SF3 SPR instrument (Sartorius)
- **Cost**: € 696,46/day (sensor chips and consumables included)

Mass Photometry

- **Service ID**: RMMP
- **Name**: label-free characterization of macromolecule samples (sample homogeneity, protein aggregation and oligomerization, biomolecular interactions, macromolecular complex assembly)
- **Description**: measurement of the light scattered by individual particles. The signal allows to count the particles and measure their mass with high accuracy.
- **Equipment**:
  - TwoMP mass photometry instrument (Refeyn)
- **Cost**: to be approved (available upon request)

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