



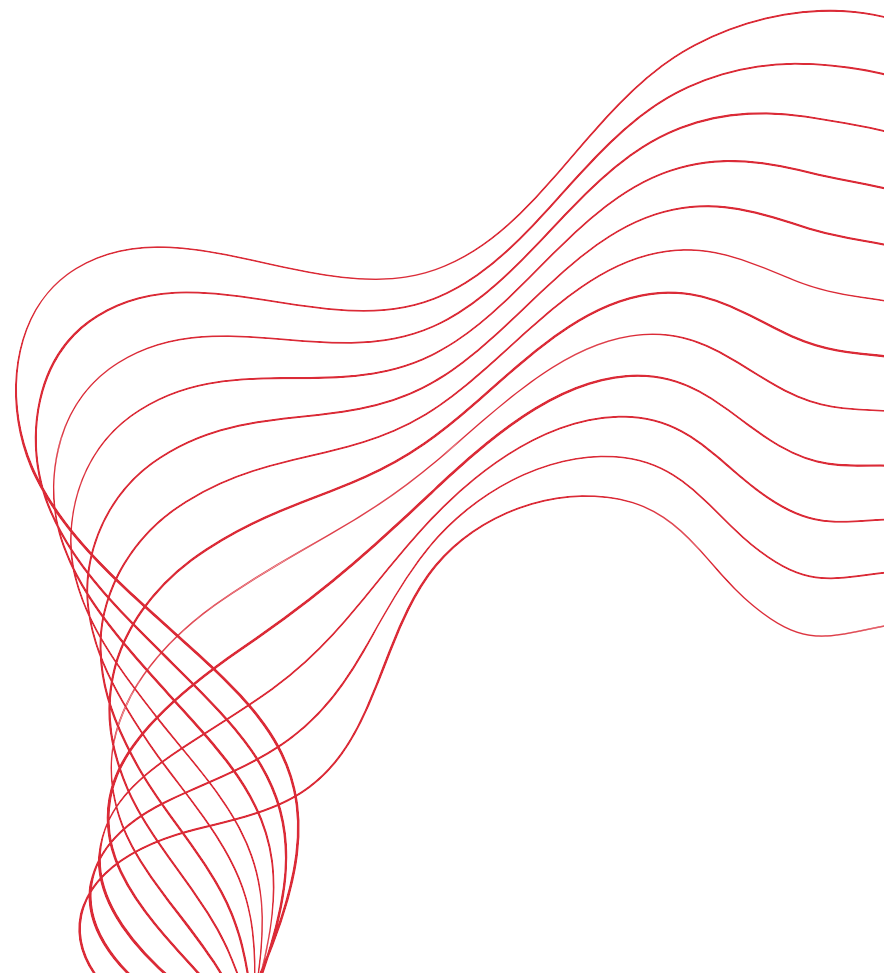
CCiTUB

Centres Científics i Tecnològics
UNIVERSITAT DE BARCELONA

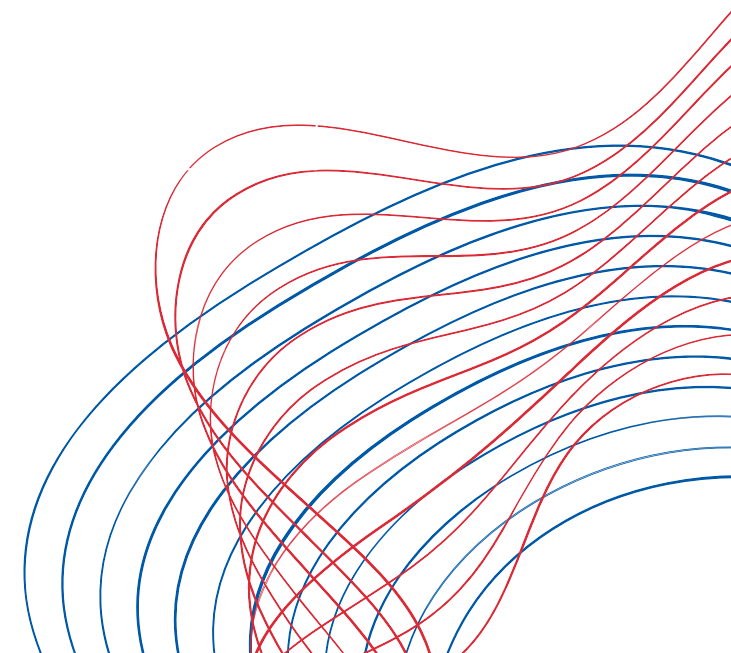
Centres Científics i Tecnològics
CCiTUB

Tècniques d'anàlisi i caracterització
avançada al servei de la recerca

Dr. Juan F. Sangüesa – Director CCiTUB



*"Promote and facilitate **research and innovation** through the provision of highly specialized and complementary experimental support services"*



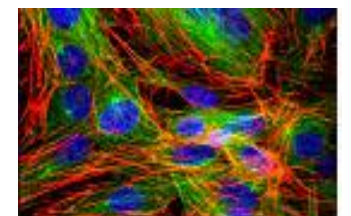
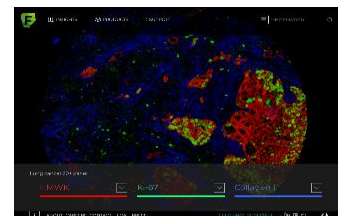
OUR OFFER

- **Expertise**

- **180 specialized technicians**
- **>30 years experience**

- **Multidisciplinarity**

- **3 main fields: Materials, Chemistry, Biosciences**
- **Broad set of complementary techniques and services**



- **Quality**



- **Excellence**



- **Integral service**



LOCATION

CCiTUB

Centres Científics i Tecnològics
UNIVERSITAT DE BARCELONA

Diagonal

- **Solé i Sabarís**

Electron Microscopy (TEM, SEM,
Microprobe, AFM, ESFOSCAN)
DRX & Therm. Analysis
GC-MS & Isotopic Analysis
Metal Analysis,
Vibrational Spect. (RAMAN, IR, CD)

- **F. Farmàcia**

NMR (medium field)
Animal Exp.
IRA

- **F. Biologia**

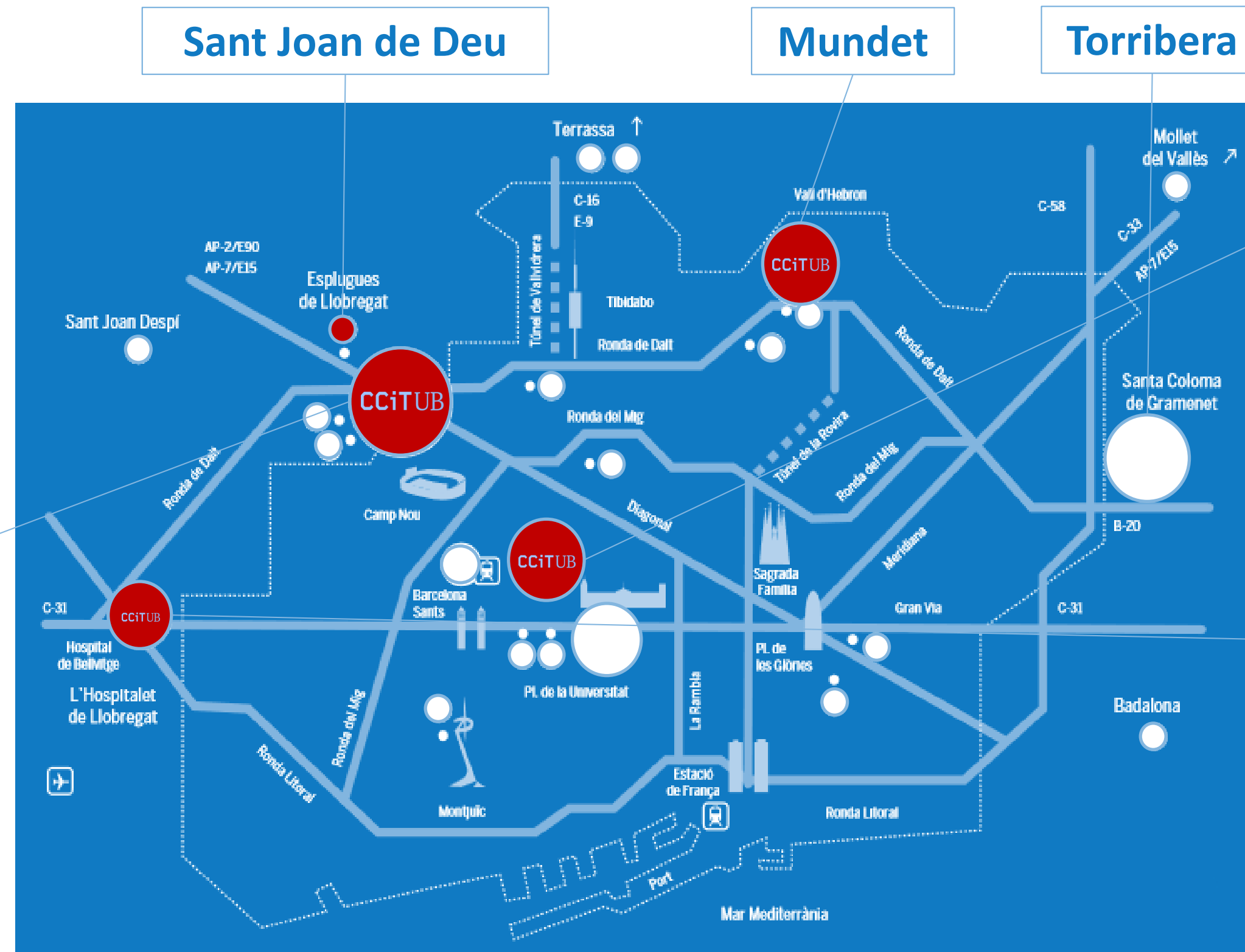
Optical Microscopy
Animal Exp. (aquatic)
IRA

- **F. Química**

NMR (medium field), EPR, SQUID
Mass Spect.
Radiocarbon
Workshop

- **PCB**

Electron Microscopy
(TEM, CrioTEM)
Genomics
Cytometry
Biomol. Analysis
(Proteomics, HPLC, Interactions)
NMR (high field)



Clínic

- **F. Medicina**

Electron Microscopy (TEM, SEM)
Optical Microscopy
Animal Exp.
IRA

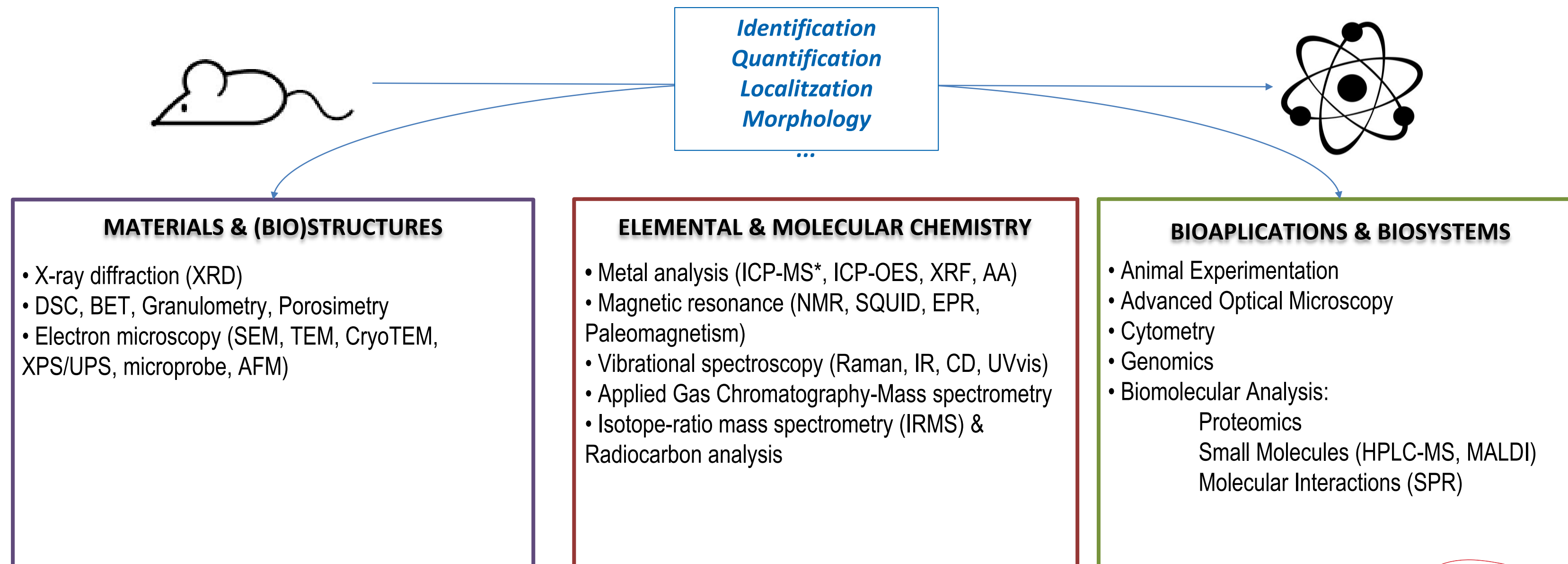
Bellvitge

- **F. Medicina**

Optical Microscopy
Cytometry
Genomics
Animal Exp.
IRA

5 locations - 12.000 m²

OUR EXPERTISE: ANALYSIS & CHARACTERIZATION

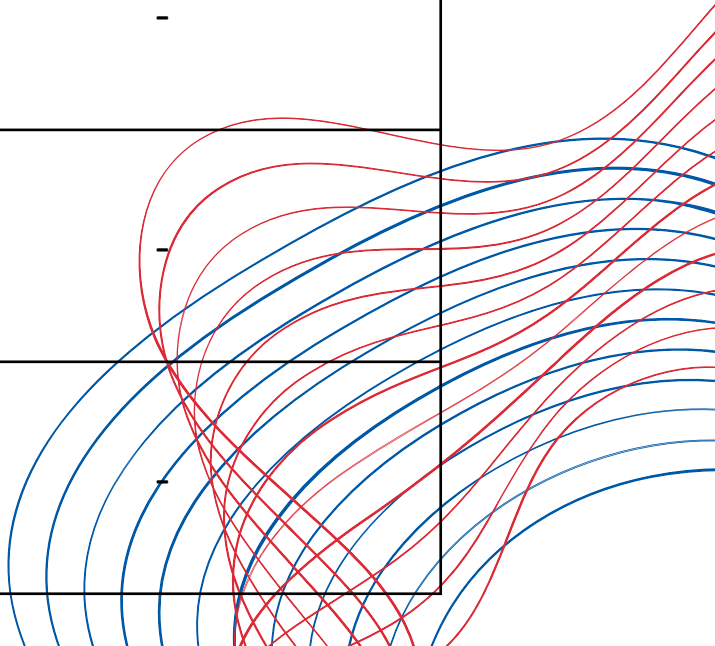


Other transversal Services:

Radiological Protection, FabLab/Workshop, Field station (ECAM)

Laboratory Animal Housing

Species	Location	Housing type	Related studies	Related AE services	Other related services
Rabbit 	Bellvitge, SJD	Conventional	Experimental	Antibody production	-
Rodents 	Diagonal, Clínic, Bellvitge, Mundet, SJD	Conventional, SPF, Negative Pressure	Experimental, Behavior	Cryopreservation	In vivo imaging, electrophysiology, irradiation
Xenopus 	Bellvitge	Conventional	Experimental	Cryopreservation	-
Fish 	Diagonal	Conventional	Experimental, Behavior	-	-
Sheep 	Bellvitge, SJD	Conventional	Experimental	Surgery room	-
Pig 	Clínic, Bellvitge	Conventional	Experimental	Surgery room	-



Featured Services & Techniques

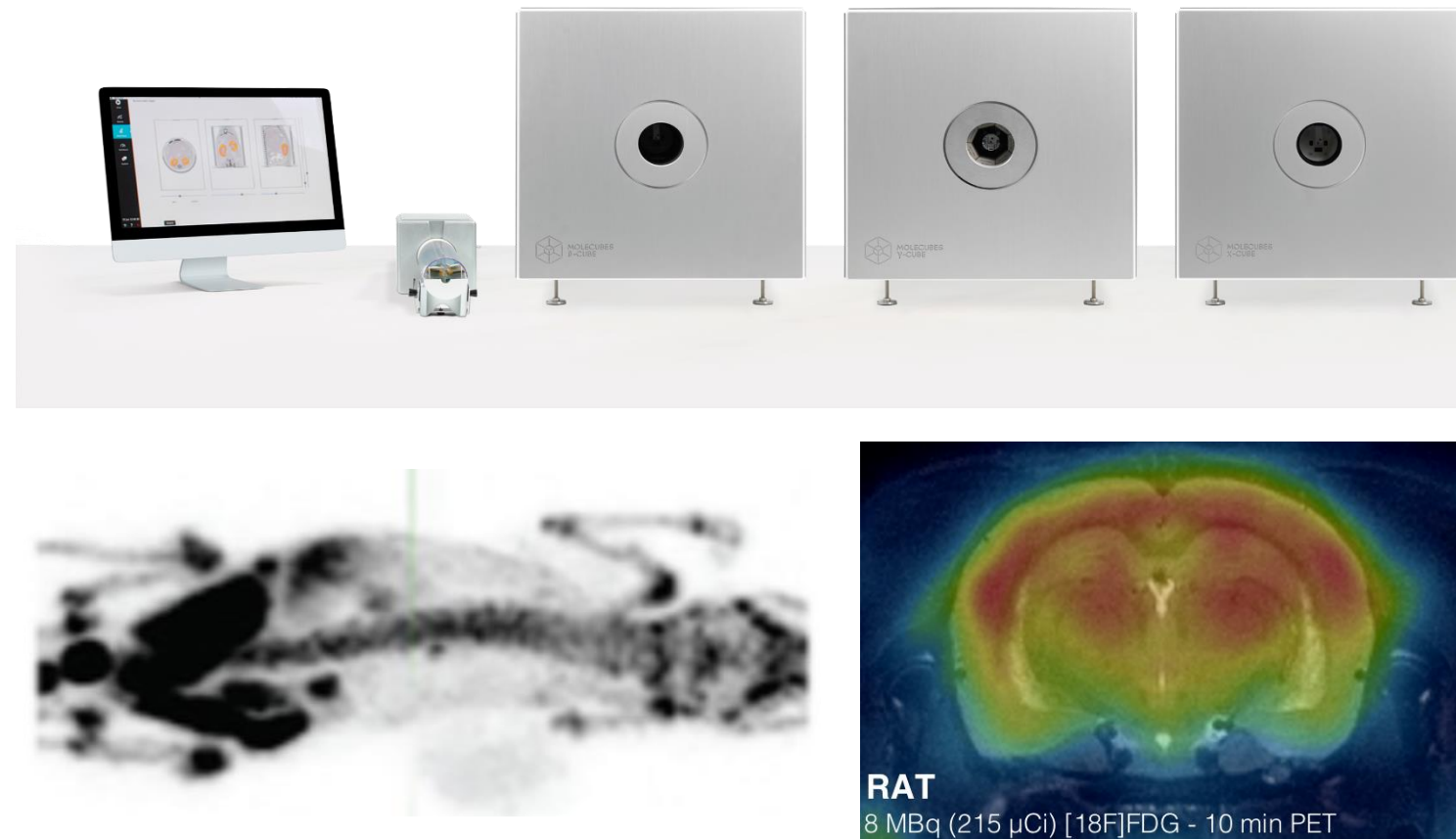
EchoMRI™-100H



Body composition analysis (fat, lean, water) for mouse/rat

Diagonal

MOLECUBES – PET/SPECT/CT

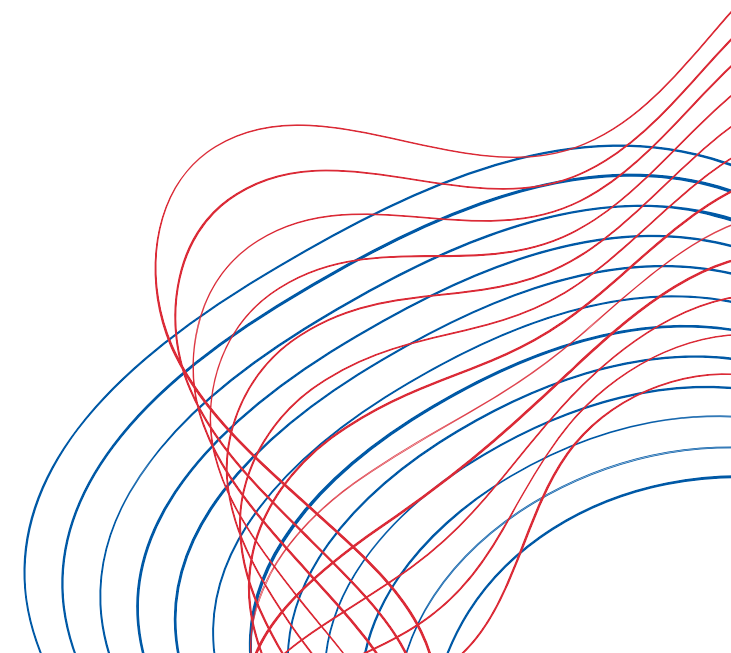


Whole-body micro-CT, micro-SPECT and micro-PET scanners for mouse/rat

Bellvitge

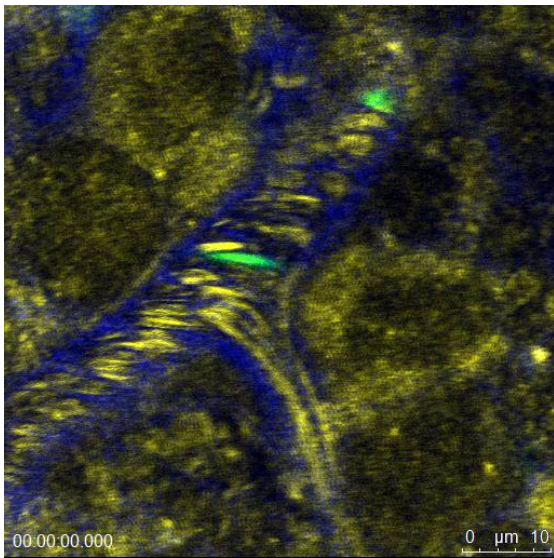
OTHER FEATURED EQUIPMENT

- Metabolic cages (*Diagonal*)
- Activity/motor measurement system (*Diagonal/Mundet*)
- Behavior study systems (Intellicage, Catwalk,...) (*Mundet*)
- In vivo electrophysiology (*Mundet*)
- Bioluminescence/Fluorescence (*Clinic*)

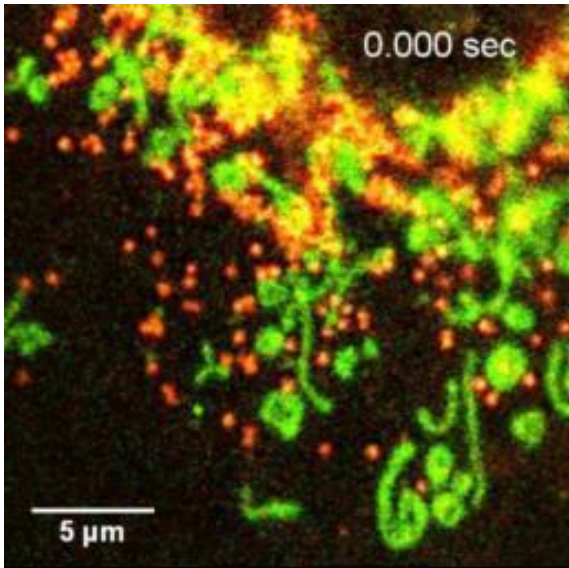


Available Technologies and Services

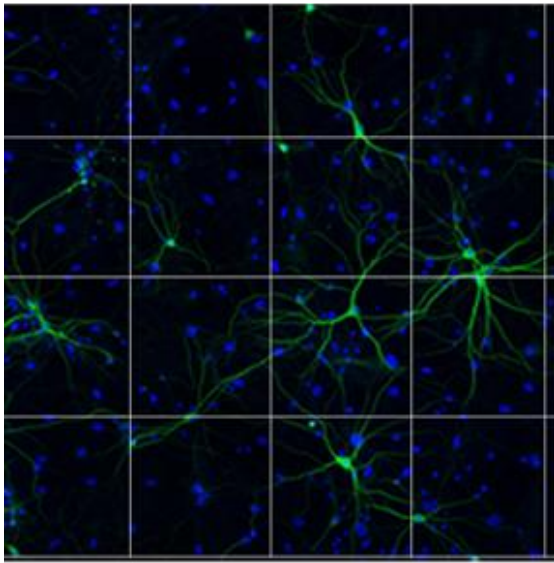
	Widefield fluorescence	Laser Scanning Confocal	Multiphoton	Bioluminescence	Image Analysis
Depth	Limited depth	Limited depth (50-100 mm)	Extended depth NIR light source (100-500 mm)	Limited depth	3 Offline Image Analysis Computer Imaris Filament Tracer, Track, Coloc, Cell, XT Metamorph, Stereo Investigator Open Source Software: ilastik, FIJI, Qpath, Cell Profiler,
Optical Section	Deconvolution required	Optical Section High spatial resolution	Intrinsic optical section (1- 1.5um)	Optical section	
Light Source	Lamp	Laser	Laser	Bioluminescence	
Detection	Camera (CCD,CMOS...) Fast acquisition	PMT Resonant scan for high speed imaging	PMT Resonant scan for high speed imaging	CCD	
Location	Diagonal, Clínic, Bellvitge	Diagonal, Clínic, Bellvitge	Clínic	Clínic	



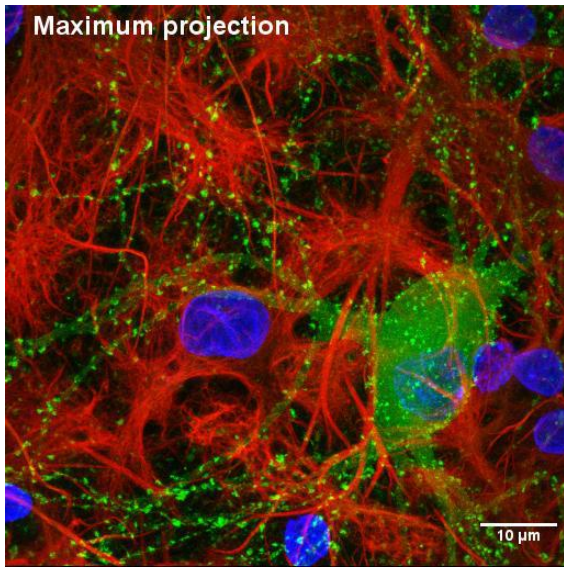
Two Photon Intravital
Microscopy



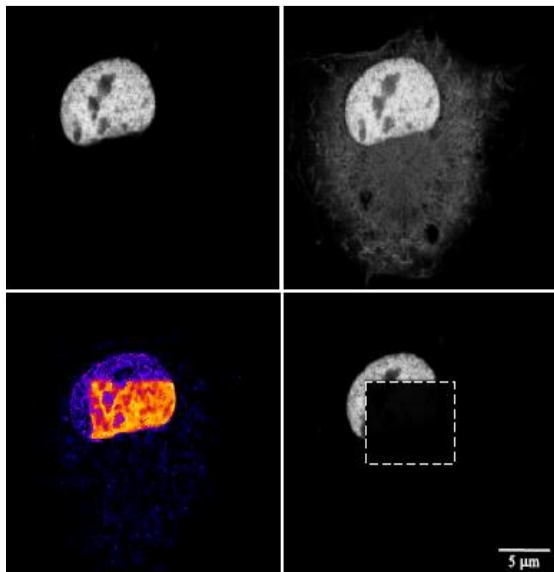
Live Cell Imaging



Automated
Microscopy



3D Imaging



FRET

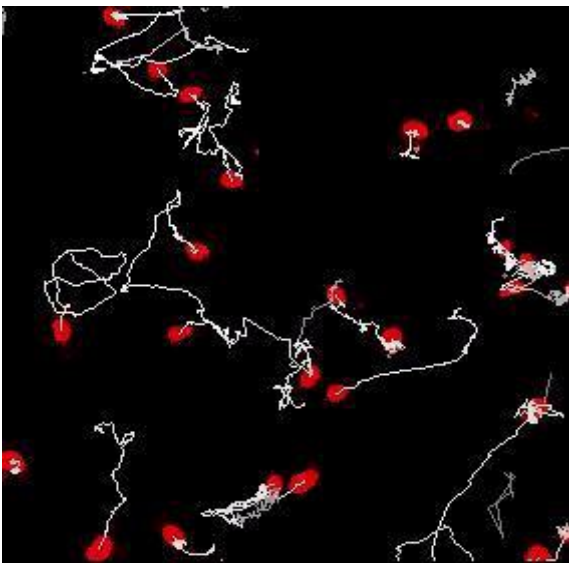
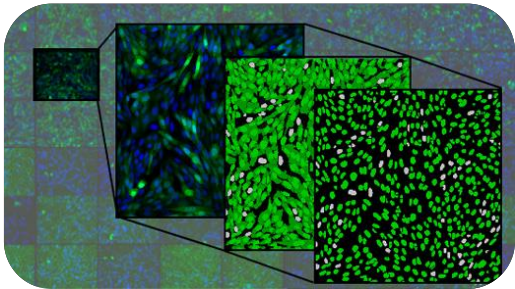
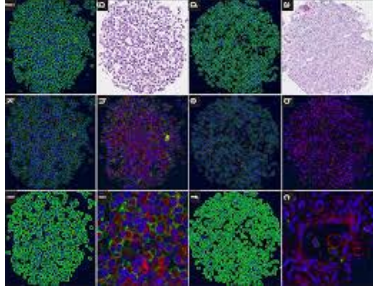
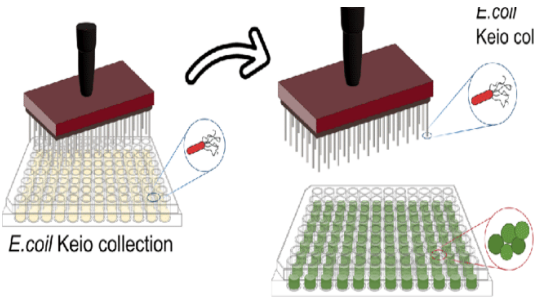


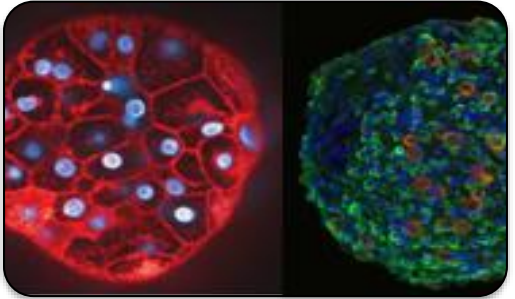
Image Analysis

Featured Services & Techniques

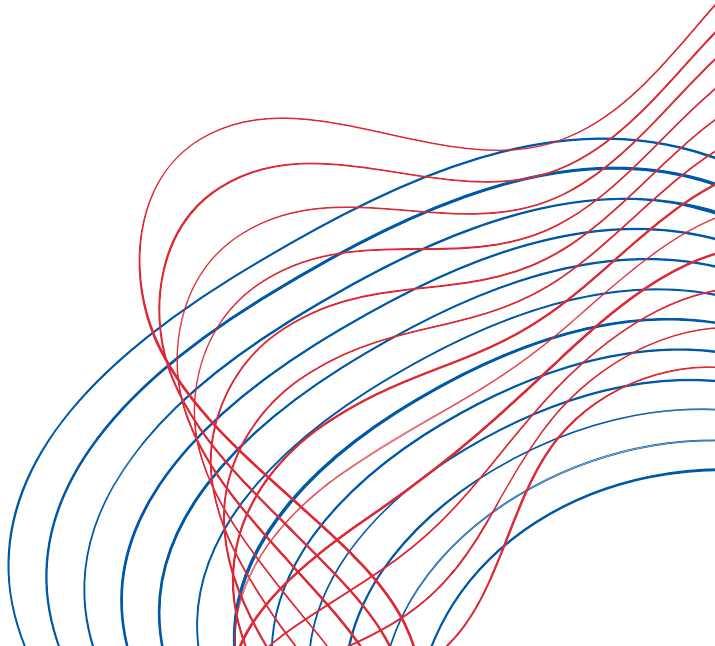
Opera Phenix™ Plus



- ### High Content Screening
- Automated Microscopy Phenotypic
 - Characterization of Cellular Populations
 - Testing of Therapeutic Compounds, siRNA Libraries, Other Molecules
 - Large-Scale Projects/Collaborations in Projects
 - Collaboration with Pharmaceutical Companies



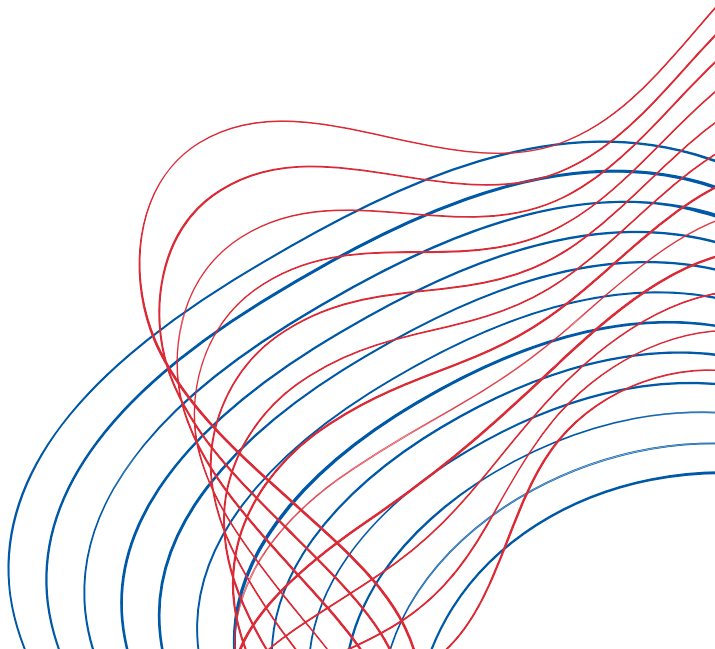
- ### Spinning Disk
- In Vivo Microscopy, Live Cell Microscopy
 - Organoids, Spheroids, 3D Cultures, Cleared Organs
 - High Sensitivity Rapid Microscopy 3D 4D: Depth and Temporal



Available Technologies and Services

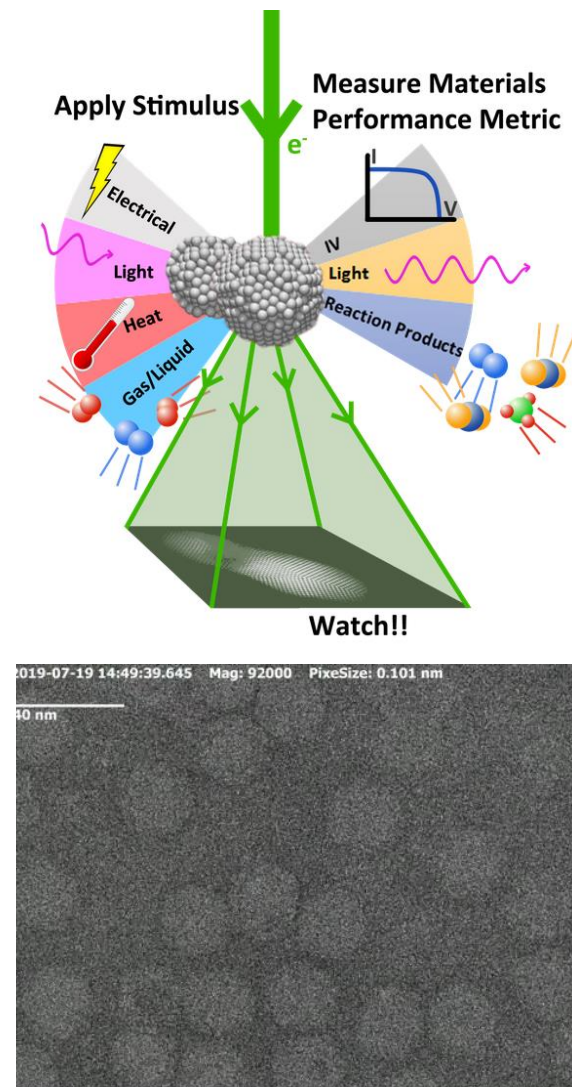
	Transmission Electron Microscopy (TEM)	(Cryo)Transmission Electron Microscopy (CryoTEM)	Scanning Electron Microscopy (SEM)	Correlative Light- Electron Microscopy (CLEM)	Dual-Beam (FIB-SEM)	Scanning transmission electron microscopy (STEM)
Applications	Ultrastructure studies	Ultrastructure studies (biological samples)	Morphological and surface studies	Subcellular localization	Tomography, 3D reconstruction	In situ studies, Ultrastructure studies
Sample preparation complexity	++ (ultramicrotomy)	+++ (cryo-preparation)	+ (conductive coating)	+++	+++	+++ (lamella preparation, in situ)
Instruments available	6	1	4	3*	1	1
Location	Diagonal, Clínic	Diagonal	Diagonal, Clínic	Diagonal	Diagonal	Diagonal

- Samples:**
- Suspensions: nanoparticles, liposomes, protein complexes, nucleic acids, virus, exosomes, isolated organelles.
 - Cells: bacteria, protists, fungi, euchariotic cell lines.
 - Little organisms: larva, worms.
 - Tissues: animal, vegetal, algae, fungi.
 - Semisolids and solids: gels, polymers.
 - Medical biopsy analysis



Featured Services & Techniques

JEOL NeoARM 200 cF



Aberration corrected (S)TEM with:

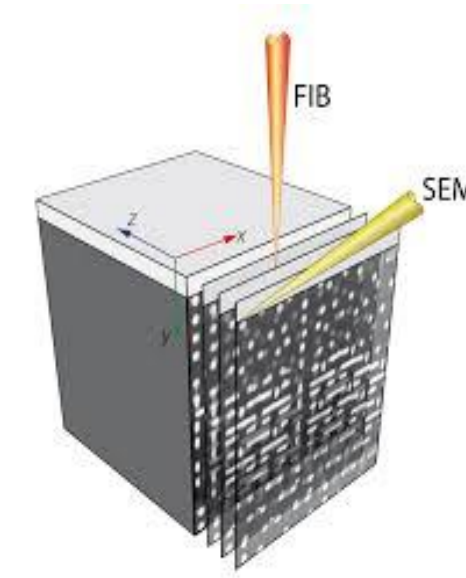
- Dose Modulator
- Sensitive and fast cameras
- EELS & EDXS spectroscopies
- **In situ stimuli:** LIQUID CELL, HEATING/COOLING, BIASING

Zeiss Crossbeam 350



FIB/SEM dual beam system with:

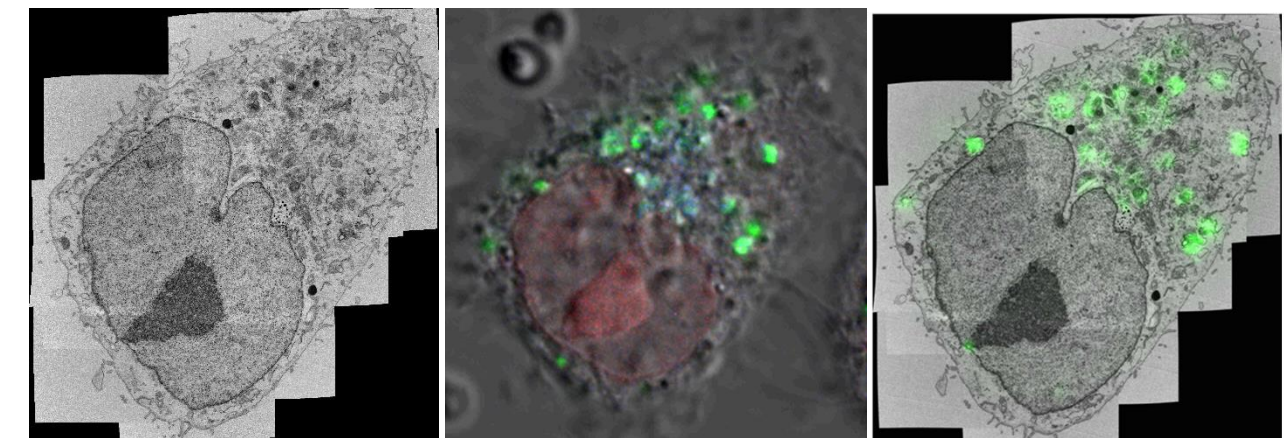
- In-chamber micromanipulator
- Cryogenic and RT work conditions



Volumetric Reconstruction



Correlative Microscopy



Available Technologies and Services

METABOLOMICS / SMALL MOLECULES

- BIODISTRIBUTION SMALL MOLECULES IN TISSUES
- PHARMACOKINETICS
- DRUG METABOLISM
- BIOMARKER DISCOVERY IN DISEASES AND NUTRITIONAL STUDIES
- DRUG DEGRADATION
- DRUG RELEASE
- AMINO ACID ANALYSIS
- HPLC QUANTIFICATION
- COMPOUND CHARACTERIZATION (ORGANIC /INORGANIC)
- EMPIRICAL FORMULA CALCULATION

PROTEOMICS

- BIOMARKER IDENTIFICATION
- PROTEIN/PROTEIN INTERACTIONS
- PROTEIN COVERAGE
- QUANTITATIVE PROTEOMICS
- QUALITATIVE PROTEOMICS
- MOLECULAR MASS
- POST-TRANSLATIONAL MODIFICATION
- DATA ANALYSIS
- PEPTIDE SEQUENCING

MOLECULAR INTERACTIONS

- FREE LABELLING MOLECULAR INTERACTIONS
- DRUG SCREENING
- TARGET VALIDATION
- AFFINITY (K_A & K_D)
- KINETICS (k_{on} , k_{off})
- HALF LIFE OF A COMPLEX. THERMODYNAMICS
- BIOSIMILAR SIMILARITY SCORE
- COMPETITIVE DRUG ASSAY
- THERMODYNAMICS
- **DATA ANALYSIS FITTED TO MATHEMATICAL MODEL**

10 Mass Spectrometers (MS) coupled on-line to UHPLC and nanoUHPLC systems

LOW RESOLUTION

(qualitative and quantitative information)



4000 QTRAP
(SCIEX)



QTRAP 6500
(SCIEX)



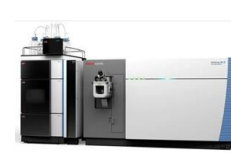
7500 QTRAP
(SCIEX)

HIGH RESOLUTION

(qualitative and quantitative information)



LTQ-ORBITRAP VELOS
(THERMO)



ORBITRAP IQ-X
(THERMO)



ION MOBILITY-QTOF
AGILENT 6560



LC/MSD TOF
(Agilent)

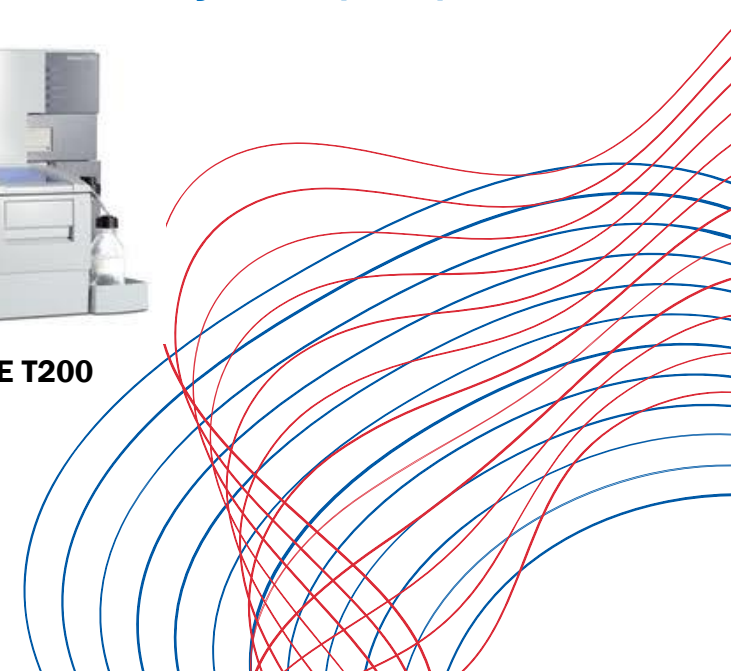
1 MALDI-TOF-TOF

4 HPLC /GPC with different detectors (UV, ...)

1 Surface Plasmon Resonance system (SPR)

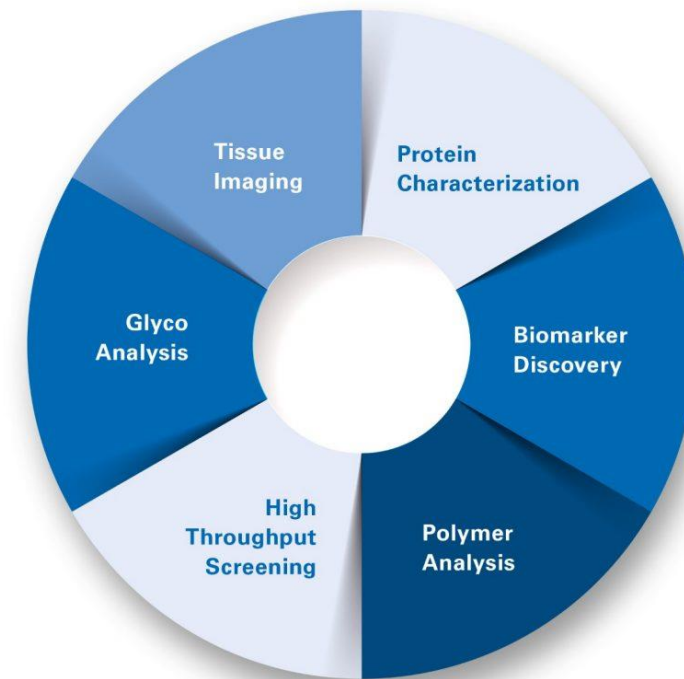


BIACORE T200

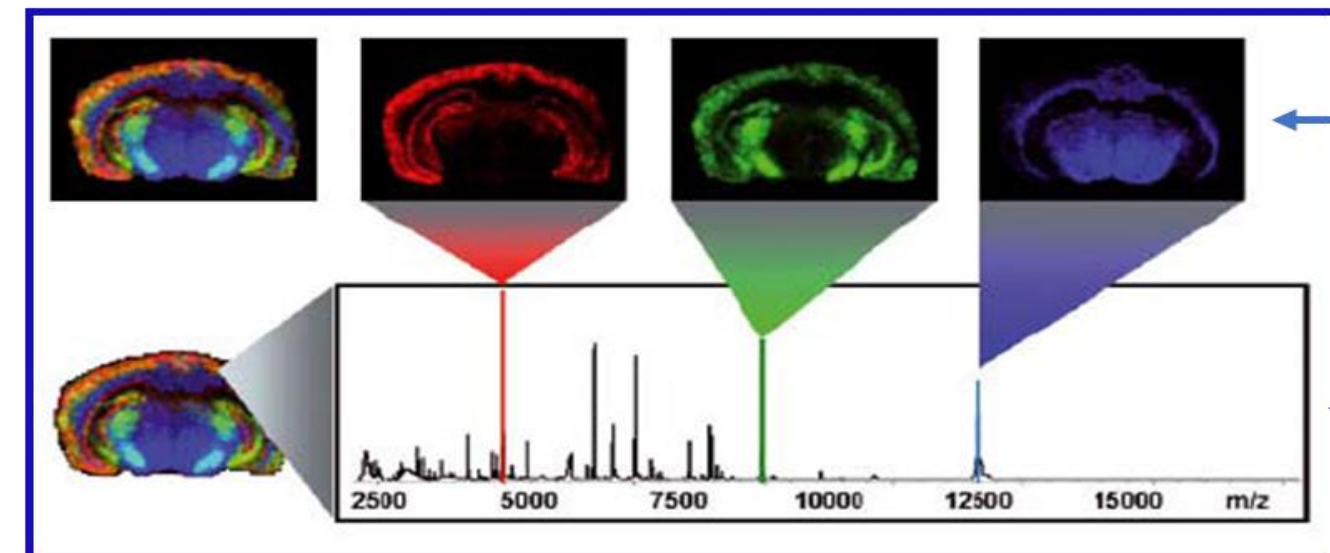


Featured Services & Techniques

BRUKER rapifleX

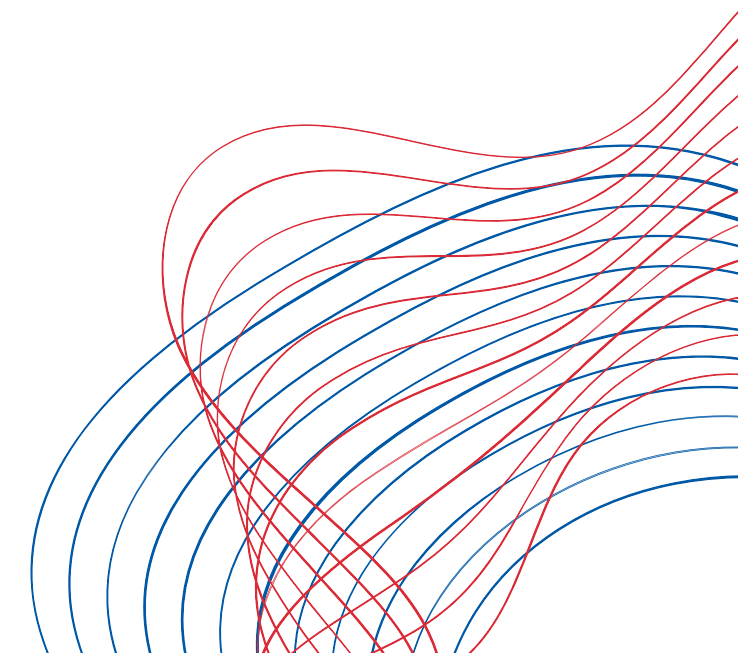


Tissue Imaging Mass Spectrometry



MALDI-TOF/TOF System for :

- In-depth protein characterization
- **MALDI Imaging**
- High-throughput screening



Available Technologies and Services

Conventional flow cytometric analysis

- 2x BCGallios3l 10c
- BD FAcscantoll 2l 6c
- BD FacsCalibur2l 4c

Diagonal, Bellvitge

Conventional sorting

- 2x BD FACS Fusion 4I 16c
- BD FACS Aria SORP 4I 18c
- BC MoFlo Astrios 4I 14c

Diagonal, Bellvitge

Spectral flow cytometric analysis

- Cytek Aurora 4l

Diagonal

Spectral sorting

- BD FACSDiscover S8
(with cell view®)

Diagonal

Soluble molecules detection

- Luminex Magpix
- Mabtech Elispot Astor

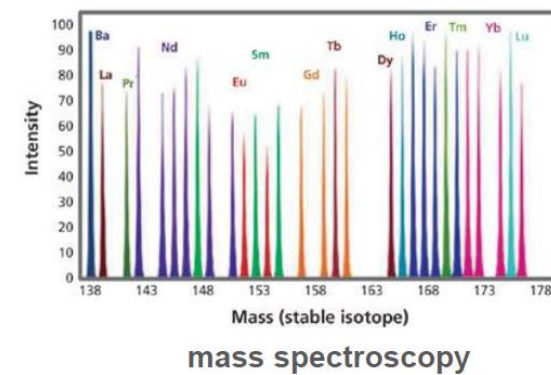
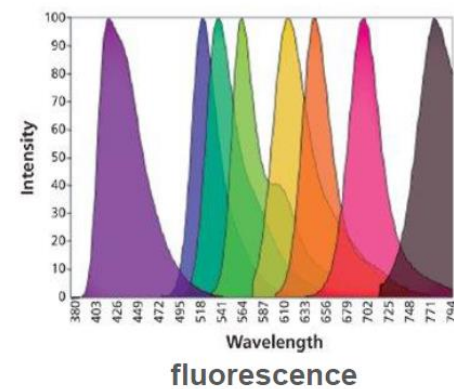
Diagonal

Mass cytometry

- Standard Biotoools

Diagonal

Fluorescence vs. mass spectroscopy:



61 catalogue metals:

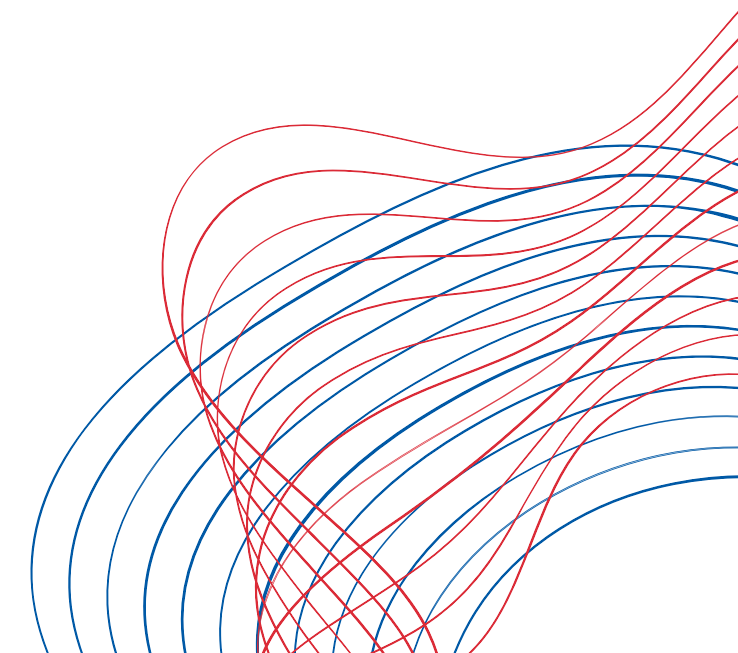
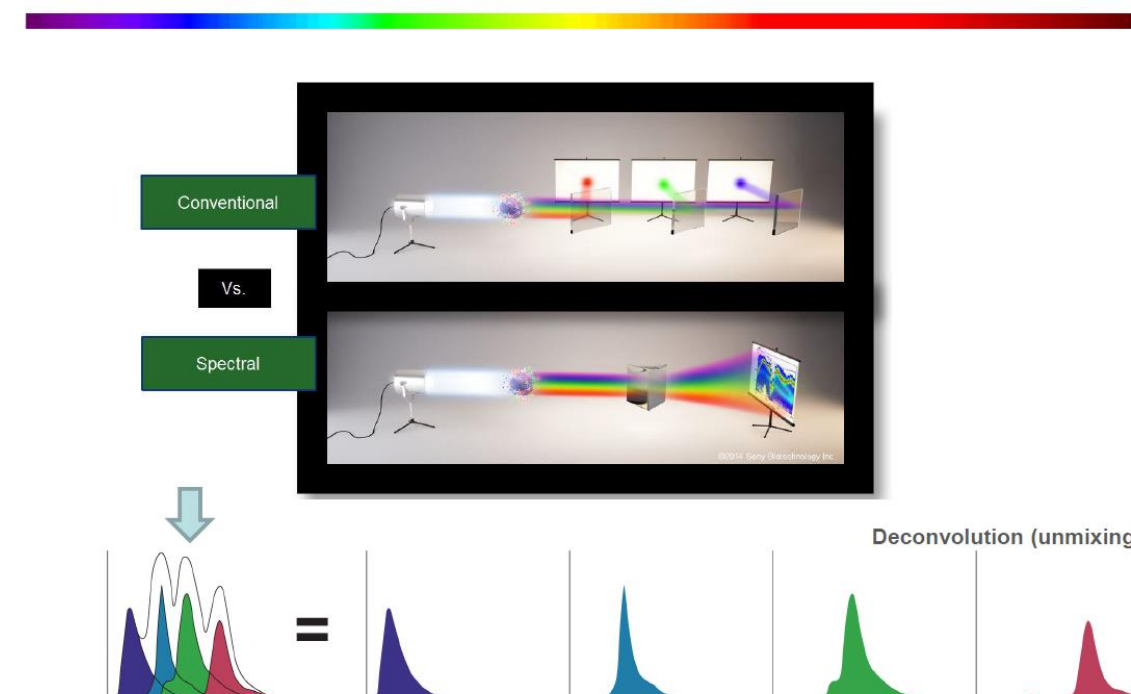
- Nonrare
- Nonbiological
- Nonradioactive



The periodic table is organized into groups and periods. The elements are color-coded as follows:

- Group 1 (Alkali Metals):** Pink (H, Li, Na, K, Rb, Cs, Fr).
- Group 2 (Alkaline Earth Metals):** Light blue (Be, Mg, Ca, Sr, Ba, Ra).
- Groups 3-10 (Transition Metals):** Yellow (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr).
- Group 11 (Coinage Metals):** Light green (Cu, Ag, Au).
- Group 12 (Zn, Cd, Hg):** Light blue.
- Groups 13-18 (Main Group Elements):** Light green (B, C, N, O, F, Ne, Al, Si, P, S, Cl, Ar, Ga, Ge, As, Se, Br, Kr, Sb, Te, I, Xe, Po, At, Rn, Fr, Ra, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr).
- Lanthanides and Actinides:** Pink (La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr).

spectral flow cytometry



Featured Services & Techniques

Helios® (Fluidigm)



Mass cytometer

- +50 marker panel
 - Speed: 500 evts /sec
 - Panel flexibility
 - Process combined samples
 - Keep cells frozen after staining
- DESTRUCTIVE

Aurora® (Cytek)

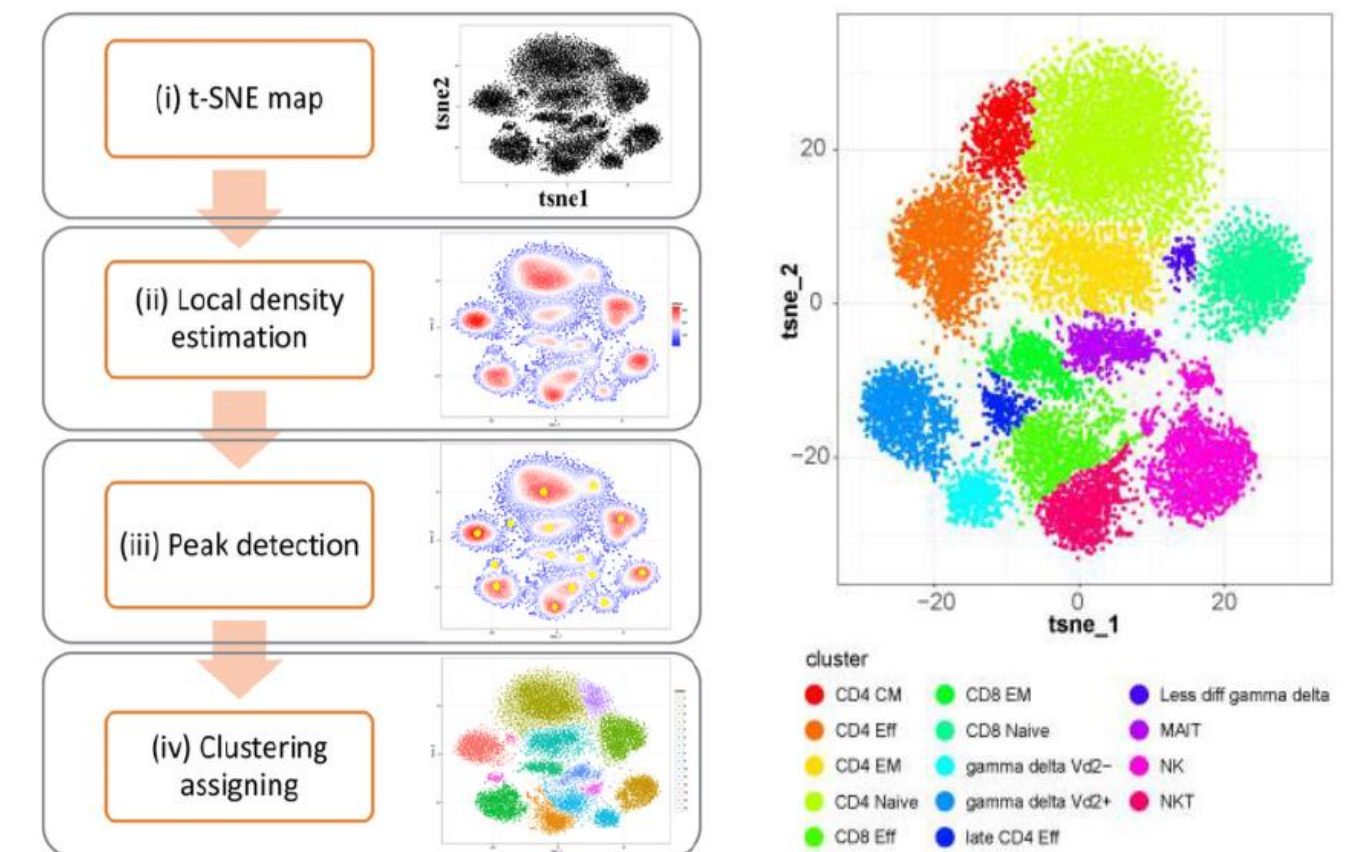


Spectral cytometer

- 45 markers panel
 - Speed: 20,000 evts /sec
 - Large projects
 - Easy to adapt antibodies from conventional FCM
 - Cell sorting
- NON-DESTRUCTIVE

Multiparametric data analysis: Bioinformatic approach: dimensional reduction software

Analysis of principal components + cluster analysis



- cluster
- CD4 CM
 - CD4 Eff
 - CD4 EM
 - CD4 Naive
 - CD8 EM
 - CD8 Naive
 - gamma delta Vd2-
 - gamma delta Vd2+
 - late CD4 Eff
 - Less diff gamma delta
 - MAIT
 - NK
 - NKT

Available Technologies and Services

Medium Field Equipment (400-500MHz) – Study of Medium/Small soluble molecules

Equips de RMN per molècules petites i mitjanes en dissolució	<u>Bruker 400 MHz Avance III HD</u>	<u>Bruker 400 MHz Avance Neo</u>	<u>Bruker 500 MHz Avance Neo</u>
Ubicació	Facultat de Química	Facultat de Farmàcia	Facultat de Química
Autoservei	NO	SI	NO
Mode funcionament	Personal tècnic	<u>Mixte</u>	Personal tècnic
Canviador/Capacitat	SI/16 mostres	SI/60 mostres	SI/24 mostres
Tipus de sonda	<u>Criosonda</u>	<u>Criosonda</u>	Sonda T amb



Bruker 500 MHz
Avance Neo



Bruker 400 MHz
Avance Neo



Bruker 400 MHz
Avance III HD

?

“Flow NMR”

Espectres de RMN 1D nuclis habituals	¹ H, ¹³ C, ¹⁹ F, ³¹ P-(dec- ¹ H)
Espectres de RMN 1D d’altres nuclis	²⁹ Si, ¹⁹⁵ Pt, ¹¹ B, ¹³³ Cs, ⁷ Li, ⁸⁵ Rb, ⁵⁵ V, ²³ Na, ³⁷ Cl
Espectres RMN 1D singulars	¹ H-(dec- ³¹ P) ¹⁹ F ¹ H-(dec- ¹⁹ F)
Espectres 1H-RMN amb eliminació d’H2O	Presaturació, watergate, excitation exculpting
Quantificació per RMN	1H-qNMR
Espectres RMN 1D sel·lectius	1D NOESY, 1D ROESY, 1D TOCSY
Espectres de RMN 2D homonuclears	¹ H- ¹ H-gCOSY 2D-TOSCY 2D-NOESY 2D-ROESY ³¹ P- ³¹ P-gCOSY
Espectres de RMN 2D heteronuclears	¹ H- ¹³ C-gHSQC ¹ H- ¹³ C-gHMBC ¹ H- ³¹ P-gHSQC ¹ H- ³¹ P-gHMBC ¹ H- ¹⁵ N-gHSQC ¹ H- ¹⁵ N-gHMBC
Determinació coeficient difusió DOSY	¹ H i ³¹ P
Determinació de T ₁	
Experiments Temperatura variable	baixa fins a 183K, alta fins 400K

Available Technologies and Services

High-Very High Field Equipment (600 MHz – 1GHz) - Study of large molecules (proteins, nucleic acids,...) and complex systems in solution

Equip de RMN per pèptids, proteïnes, biomolècules i sistemes complexos en dissolució	<u>Bruker 600 MHz Avance III</u>	<u>Bruker 800 MHz Avance Neo</u>	<u>Bruker 1000 MHz Avance Neo**</u>
Ubicació	PCB	PCB	PCB
Autoservei	SI	SI	SI
Mode funcionament	<u>Mixte</u>	<u>Mixte</u>	<u>Mixte</u>
Canviador	NO	NO	NO
Tipus de sonda	<u>Criosonda</u>	<u>Criosonda</u>	<u>Criosonda</u>
Experiments 2D ¹ H, ¹⁵ N-HSQC 2D-NOESY 3D ¹ H, ¹⁵ N-HSQC-TOCSY 3D HNCA 3D HNCACB 3D ¹ H, ¹⁵ N-HSQC-NOESY	SI	SI	SI
Prestacions			
Caracterització estructural de pèptids i proteïnes globulars Experiments 3D de triple ressonància. TROSY	SI	SI	SI
Caracterització de proteïnes intrínsecament desordenades	SI	SI	SI
Estudi de sistemes dinàmics per RMN: <u>drug-design</u> tant per proteïnes globulars com desordenades; caracterització de la dinàmica de proteïnes per relaxació	SI	SI	SI
Estudis de sistemes complexos de biomolècules	SI	SI	SI



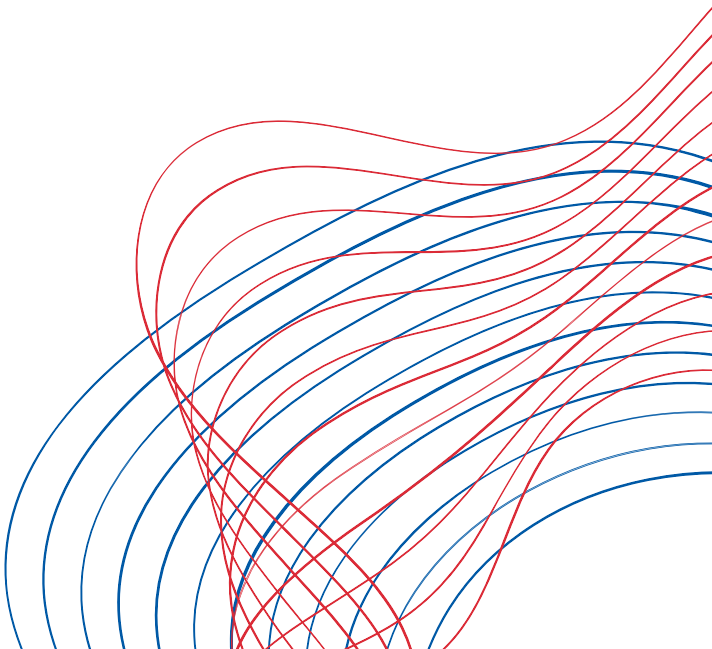
Bruker 1000 MHz
Avance Neo



Bruker 600 MHz
Avance III



Bruker 800 MHz
Avance Neo



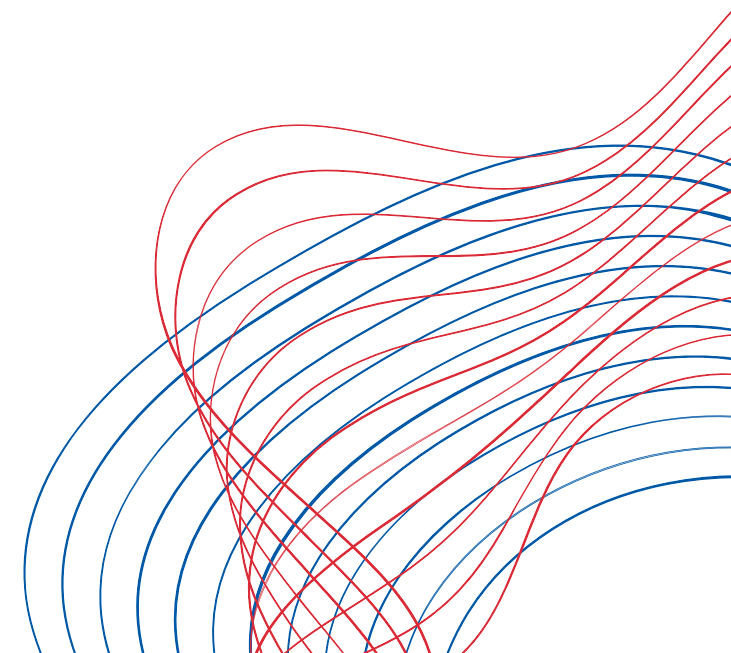
Featured Services & Techniques

Bruker 1000 MHz Avance Neo



New drug targets

“Biologics” characterization



Available Techniques and Services

TECHNIQUES

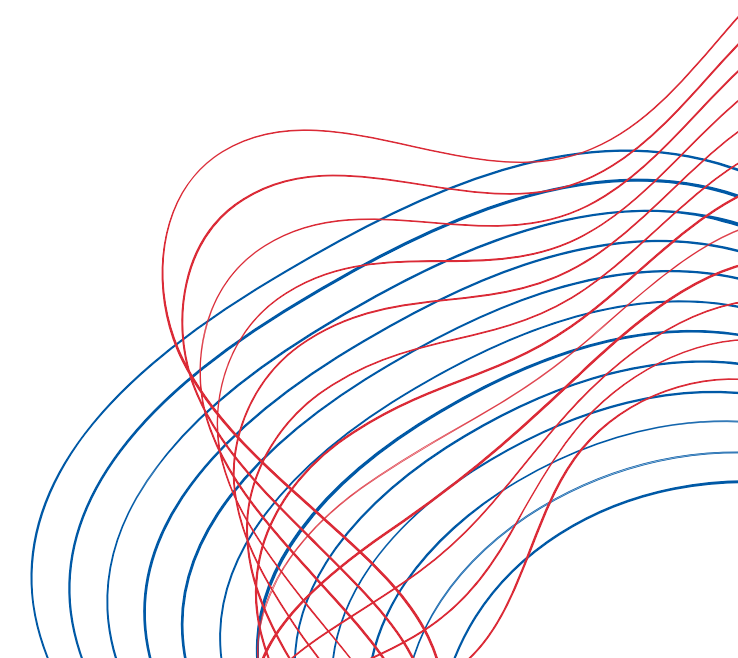
- ✓ CG gas chromatography with FID, ECD, TCD detectors
- ✓ CG coupled to GC-MS mass spectrometry (EI, CI)
- ✓ CG coupled to isotopic ratio mass spectrometry (GC-C/Pyr-IRMS)
- ✓ Organic elemental analysis (NCHS,O)
- ✓ Elemental analysis coupled to isotope ratio mass spectrometry (EA-IRMS)

APPLICATIONS

- ✓ Characterization of active ingredients, identification of impurities
- ✓ Residual solvents (active ingredients, additives, formulations, etc.)
- ✓ Studies of molecular biomarkers (targeted metabolomics)
- ✓ Extractable compounds in different materials (biomedical devices, packaging, etc.) due to regulatory requirements
- ✓ Natural products (terpenes, alkaloids)
- ✓ Oils and fats (fatty acids, sterols, glycerides)
- ✓ Traces of organic contaminants
- ✓ Multiisotopic profiles (^{13}C , ^{15}N , ^{34}S , ^{18}O , ^2H) for characterization of origin and history, authentication of natural products, metabolomics and fluxomics studies

RELATED SERVICES

- ✓ Identification and quantification of thermostable volatile and semivolatile organic compounds in very diverse matrices. Method validation.
- ✓ Mass spectrum (EI) of pure compounds, liquids or semivolatile solids
- ✓ Isotopic analysis of specific compound (^{13}C , ^{15}N , ^2H) of volatile and semivolatile organic compounds (FAMEs, amino acids, hydrocarbons, contaminants..) with high precision and in various matrices
- ✓ Organic elemental analysis (NCHS,O)
- ✓ Elemental and isotopic analysis (^{13}C , ^{15}N , ^{34}S , ^{18}O , ^2H) in total sample (solids/liquids)

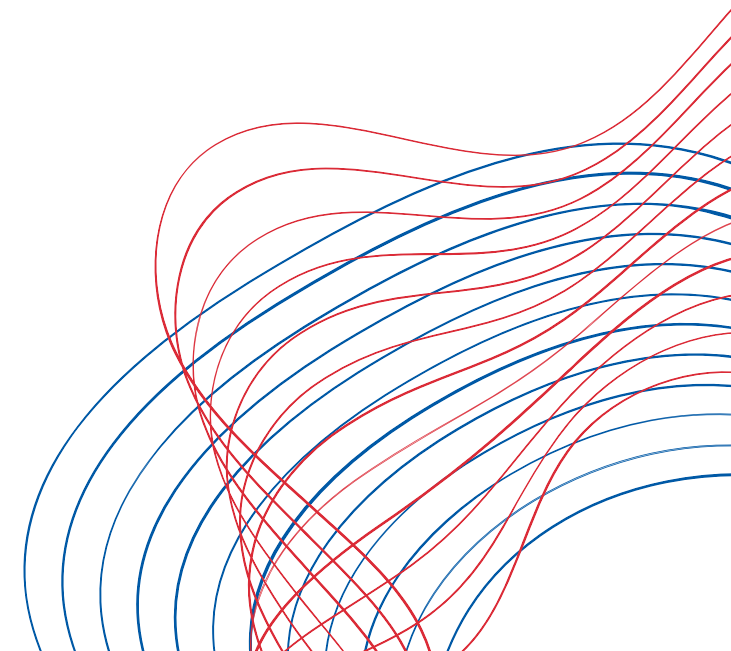


Featured Services & Techniques

GC/MS2(TQ) – *soon available*



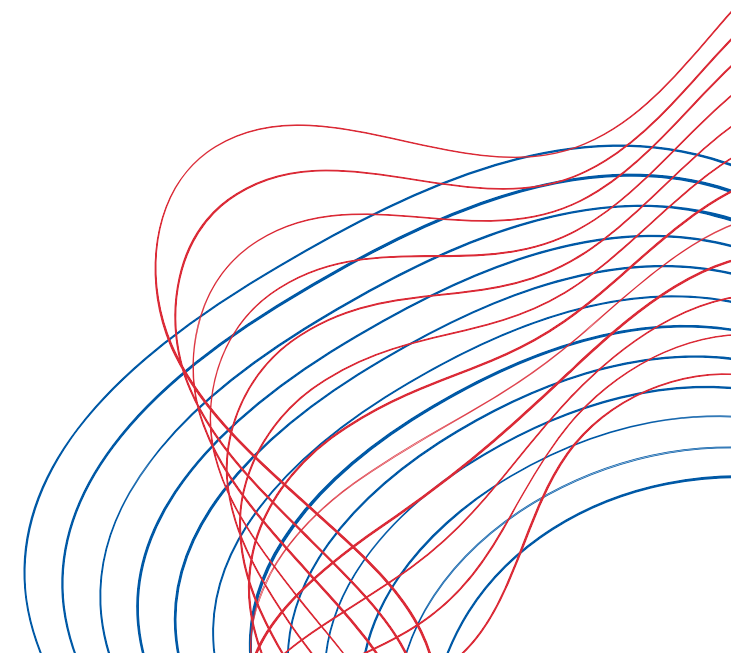
- ✓ Lower detection levels in more complex matrices (physiological, environmental, etc.)
- ✓ Powerful software to process large amounts of multicomponent data (targeted metabolomics, environmental monitoring, etc.)



Available Technologies and Services

APPLICATIONS

- ✓ Determination (solution and refinement) of crystal structures by X-ray single crystal
- ✓ Crystallinity analysis
- ✓ Qualitative phase analysis
- ✓ Semi-quantitative and quantitative analysis of crystalline phases (and eventually of amorphous phases)
- ✓ Isostructurality, isomorphism and solid state miscibility studies
- ✓ Phase analysis in depth in thin film samples (grazing incidence analysis)
- ✓ Polymorphism / pseudo-polymorphism studies
- ✓ Thermo-diffractometry: phase transitions; solid state reactions, ...
- ✓ Full profile analysis of powder diffraction data
- ✓ Rietveld method: quantitative phase analysis; crystallographic characterizations, (resolution) and refinement of crystal structures
- ✓ Microstructure analysis: crystal size analysis; microstrain; ...
- ✓ Thickness, rugosity and density of thin film materials by X-ray reflectometry
- ✓ Texture and preferred orientation analysis
- ✓ Residual stress determination
- ✓ Strain / relaxation states determination between film and substrate of hetero-epitaxial thin films
- ✓ Composition determination of hetero-epitaxial thin films of semiconductors
- ✓ Single crystal orientation determination

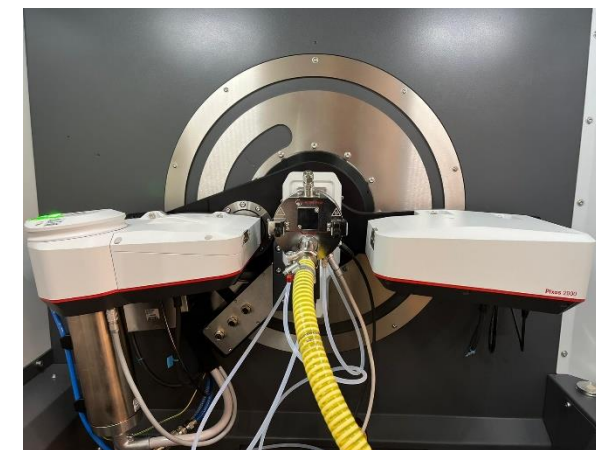


Featured Services & Techniques

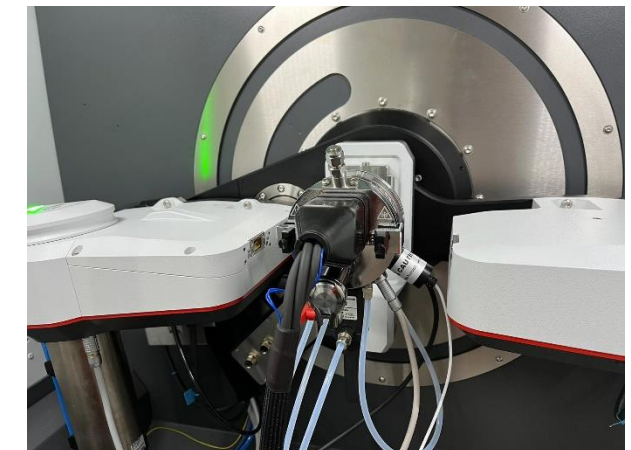
Anton Paar XRDynamic 500 multipropose diffractometer



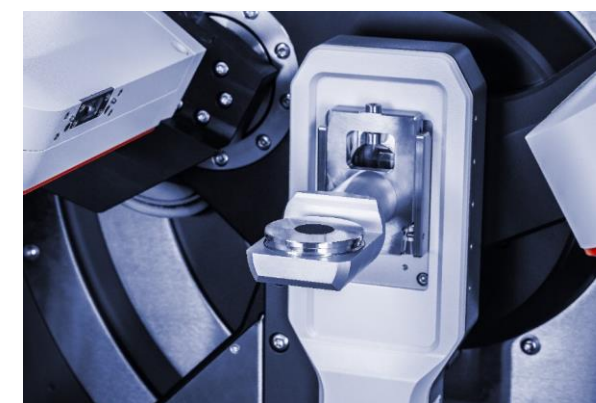
- Cu K α ($\lambda = 1.5418 \text{ \AA}$) radiation. Bragg-Brentano θ/θ Ni filtered or BB flat monochromator.
- Radius 360 or 400 mm. Evacuated incident and diffracted beam paths
- **Parabolic mirror incident parallel beam optics / Focusing elliptic mirror transmission geometry**
- CHC+ chamber; (SAXS) EVAC module
- 1D Pixos 2000 photon counting detector (**act. length 3.347°**)



Air cooling and heating modes.
Vacuum ready



Humidity mode.
+ humidity generator + humidity sensor



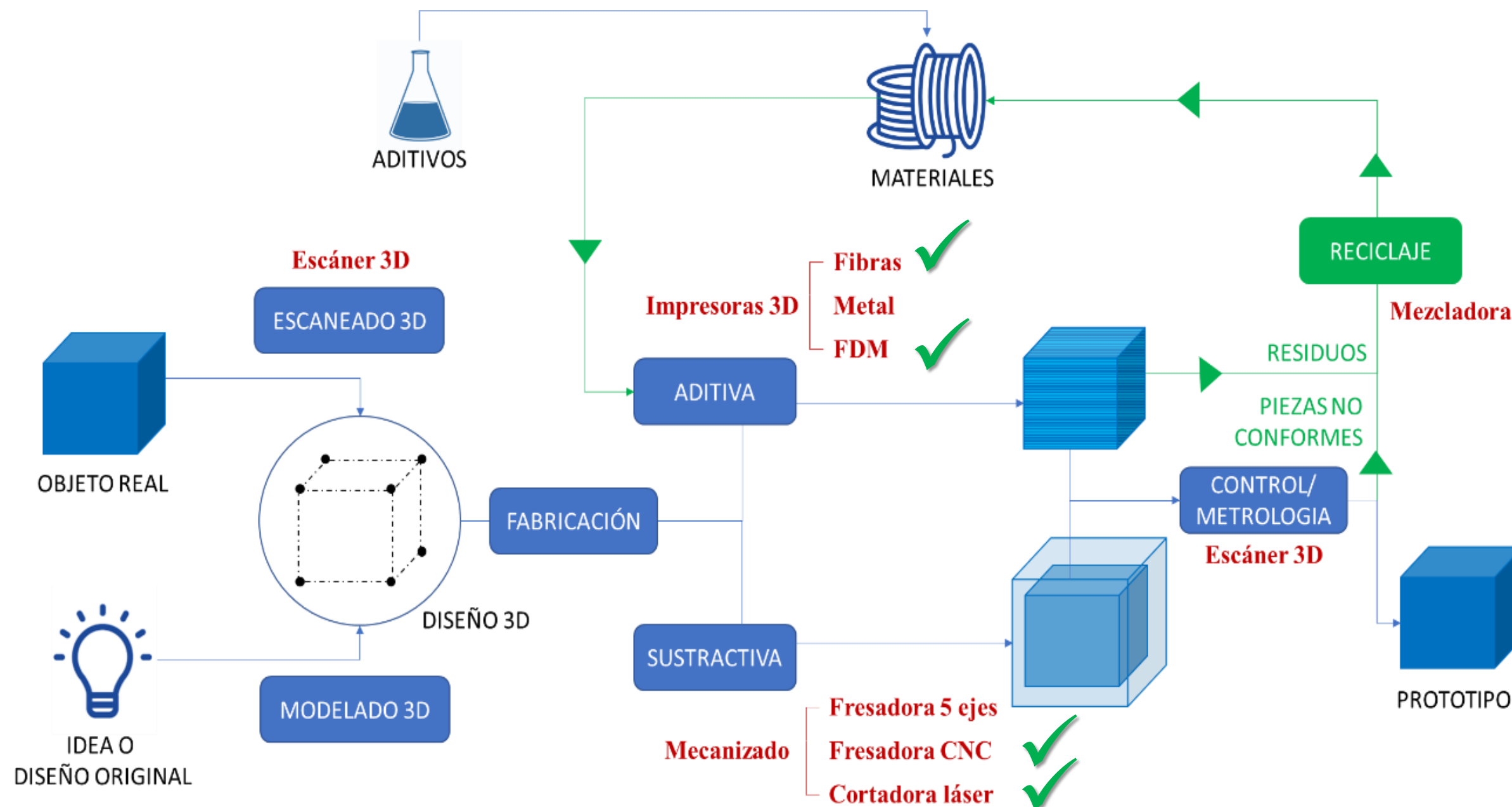
Bragg-Brentano / GID
Standard sample holder
Spinner sample holders



EVAC module, 400 mm radius,
95% evacuated
Parallel beam, Focalizing
mirror, B-B SAXS, $q_{\min}=0.05$
nm⁻¹, ($D_{\max}=60 \text{ nm}$)

Available Technologies and Services

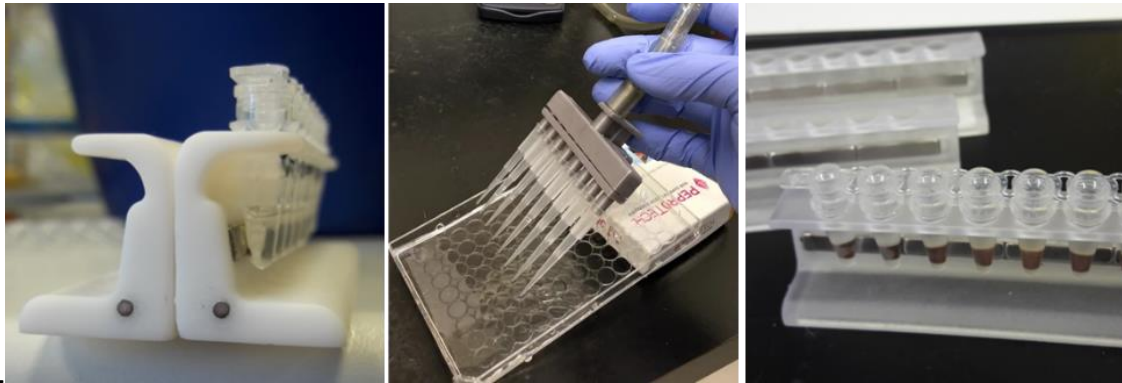
- Design and fabrication of add-ons and prototypes



Featured Services & Techniques

Design and manufacture of tools and prototypes to facilitate and enhance research activities

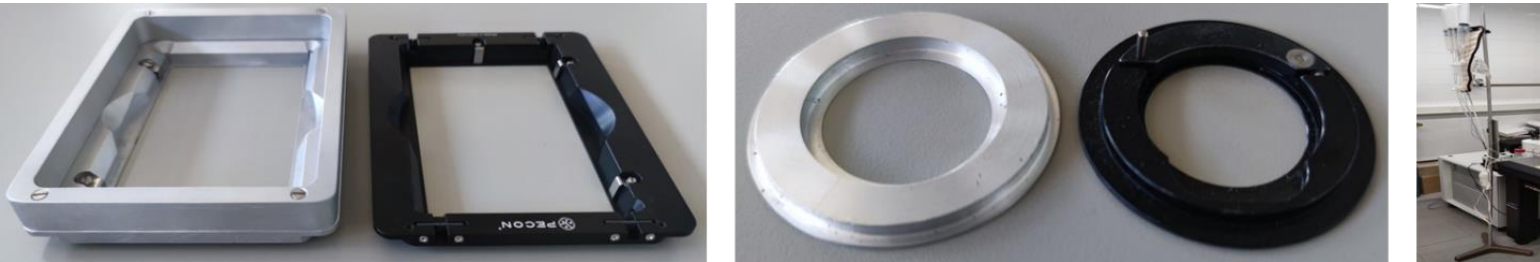
- Eines de laboratori personalitzades



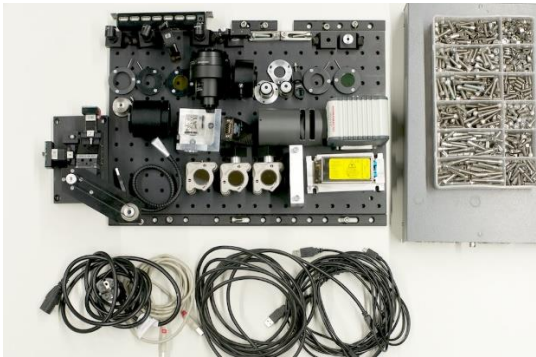
1

Exemples d'eines personalitzades per un laboratori de Biologia Molecular fabricades per impressió 3D.

- Components i complements per equipaments i instrumentació científica

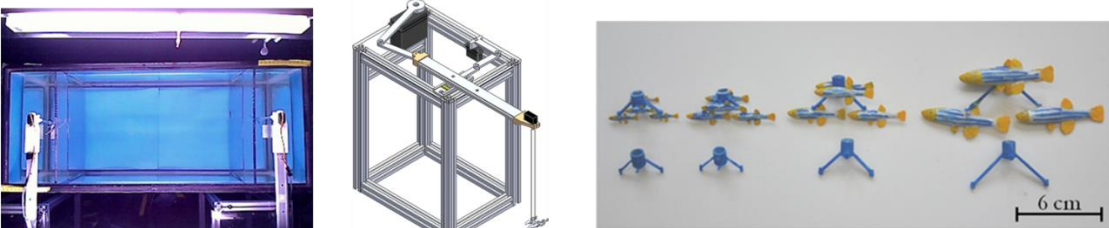


Adaptadors i sistema d'administració de productes per microscopi confocal fabricats als tallers dels CCiTUB



Components per fabricar un microscopi SPIM (Selective Plane Illumination Microscopy, [OpenSPIM](#))

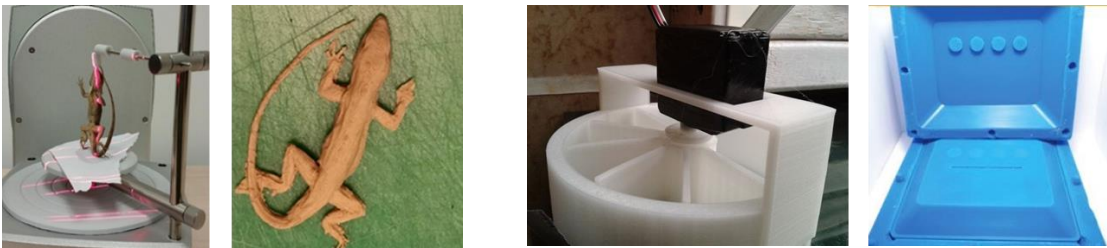
- Dispositius per estudis amb models animals (comportament, fisiopatologia, ...)



Dispositiu per estudis comportamentals de zebrafish ([Bartolini et al. 2016](#))



Dispositiu bloquejador per ratolí dissenyat i fabricat per impressió 3D als tallers del CCiTUB



Esquerra: Model de *Anolis sagrei* fabricat per impressió 3D i utilitzat en estudis de camp sobre depredadors ([Behm et al. 2018](#)).
Dreta: Distribuidor automàtic de menjar i suport per sensors per aqüicultura fabricats per impressió 3D.



www.ccit.ub.edu

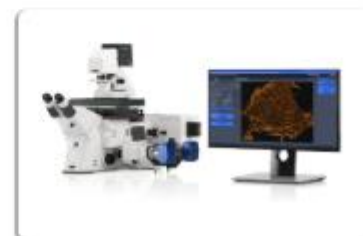
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Actualitat [\[+\]](#)



Inauguració del nou
microscopi
NeoARM Jeol



Demo: ZEISS Lattice
SIM 5

