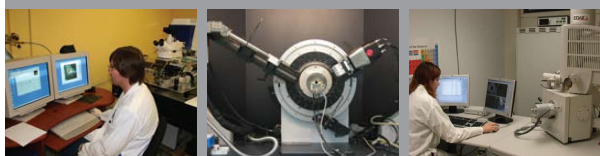


- ANALYTICAL SERVICES
- MOLECULAR SYNTHESIS

MOLECULAR CHARACTERIZATION AND SYNTHESIS CENTER

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XRD

WAXS

SAXS

NMR

AFM

STM

ESEM

TEM

LC-MS

MALDI-TOF

GC-MS

HPLC

GPC

LS

DSC

TGA

TGA-MS

DMA

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MOLECULAR SYNTHESIS AND CHARACTERIZATION CENTER

	Analytical techniques	Typical applications	Resolution / Sensitivity /	Depth resolution	Lateral resolution	Other characteristics
X-RAY DIFFRACTION	Powder diffraction <i>Bruker D8 Advance and Discover</i>	Organic and inorganic identification, quantitative analysis of crystallinity	Ang. res: 0.008° Sensitivity: 1 - 5 %	2 nm - 30 µm	0.1 - 0.5 mm	T = -176 - 450 °C Small angle measurement
	2D Diffraction/µ-diffraction <i>Bruker D8 Discover HTS</i>	High-throughput analysis of crystalline samples with µm-scale resolution	Angular res: 0.01° Sensitivity: 1 %	2 nm - 30 µm	50 µm - 0.5 mm	Multi-sample high-throughput analysis Reflection and transmission
	Single-crystal diffraction <i>Bruker Microstar (CuKa); APEX II (MoKa)</i>	Crystal structure determination	Atomic resolution	-	-	System allows study of crystals that are air-sensitive or very small (0.01 - 0.1 mm)
MASS SPECTROMETRY	LC-TOF <i>Agilent LC-MSD TOF</i>	Accurate mass, isotope ratio, chromatographic separation	10 000 at m/z 900 10 ng/mL	-	-	Ionization sources: ESI, APCI and APPI Mass range: m/z 50 - 5000
	LC-ion trap <i>Thermo Fisher LC-LCQ</i>	Structural information based on MS ⁿ fragmentation, chromatographic separation	1 000 at m/z 900 10 ng/mL	-	-	Ionization sources: ESI and APCI Mass range: m/z 50 - 2000
	Prep LC-MS <i>Thermo Fisher prepLC-MSQ</i>	Nominal mass, fraction collection triggered by mass, UV signal or time, purity assessment	1 000 at m/z 900 10 ng/mL	-	-	Ionization sources: ESI and APCI Mass range: m/z 50 - 2000
	LC-MS (triple quad) <i>Thermo Fisher LC-Quantum Ultra</i>	Structural information based on MS/MS fragmentation, chromatographic separation	5 000 at m/z 900 0.1 ng/mL	-	-	Ionization sources: ESI and APCI Mass range: m/z 50 - 1500
	MALDI-TOF <i>Bruker Daltonics Auto Flex</i>	Nominal mass, intact protein mass, average mass and polydispersity of synthetic polymers	5 000 at m/z 900 1 pmol	-	-	Operation options: linear and reflectron, positive and negative Mass range: m/z 50 - 500 000
NUCLEAR MAGNETIC RESONANCE	Solid State NMR <i>Bruker AV600WB; AV400WB</i>	Structure determination, molecular dynamic, intra-/inter-molecular interaction	Nucleus-dependent	-	-	T = -100 - 200 °C Double/Triple resonance
	NMR Imaging <i>Bruker AV600WB; AV400WB</i>	Imaging Transport phenomena (diffusion, flow)	-	> 100 µm (sample thickness)	> 10 µm (usually 100 µm)	T = -80 - 60 °C
	Liquid State NMR <i>Bruker AV700, AV500, AV400</i>	Structure determination, molecular dynamic, intra-/inter-molecular interaction	S/N 2900 (¹³ C - AV700)	-	-	Cryoprobe Double/Triple resonance
THERMAL ANALYSIS	DSC <i>Perkin DSC 7; TA (Q1000, Q2000, 2910); Mettler Toledo 823e</i>	Heat capacity, T _g , phase changes, melting, crystallization, product and oxidative stability	-	-	-	
	TGA and TGA-MS <i>TA TGA 2950; TA TGA Q500 - Pfeiffer Thermo-star GSD 301T</i>	Mass changes vs time and temperature, identification of volatile degradation compounds	mass: 0.1 mg; T: ~ 0.1°C; MS: 0 - 300 amu	-	-	MS and FTIR modules
	Mechanical measurements <i>TA DMA 2980, DMTA V, Mach 1, Instron</i>	Thermo-mechanical analysis of viscoelastic properties of solid materials	Step resolution from 0.05 µm to 0.18 µm	-	-	Static and dynamic mode Load cell from 150 g to 50 kg
MICROSCOPY	TEM <i>JEOL JEM-2011</i>	Ultrastructural analysis, diffraction and immunocytochemical characterization	-	-	0.194 nm	80-200 kV, 50-1.5M X LaB6 emitter
	FEG SEM / EDS <i>JEOL JSM-7400F / EDS</i>	Nanoscale surface imaging, elemental microanalysis and mapping	1 atomic % (EDS)	-	1.0 nm at 15 kV 1.5 nm at 1 kV	0.5-30 kV, 25-650 000 X Cold field-effect emitter, BSD
	LV SEM <i>JEOL JSM-6460LV</i>	Conventional and/or variable-pressure surface imaging of dry or wet samples	-	-	3.0 nm	0.3-30 kV, 5-300 000 X W filament emitter
	ESEM / EDS <i>FEI Quanta 200 FEG</i>	Imaging, mapping and elemental microanalysis	0.1 - 1 at%	0.5 - 3 µm (EDS)	2-5 nm (SEM) 0.3 µm (EDS)	Peletier heating/cooling & hot stages (1000°C) ETD, GSED, BSD and LFD
	AFM/STM <i>JEOL JSPM-5200</i>	Topography, phase imaging (contact, non-contact and tapping) in air and vacuum	-	0.01 nm	AFM: 0.1 nm STM: At. res.	Pressure range: atm - 10 ⁻³ Pa T range: 130 - 773 K
	Confocal microscopy <i>Zeiss LSM 510 META</i>	Intracellular distribution of molecules, fluorescence intensity and fluorophore spectra	one photon	≥ 350 nm	≥ 250 nm	Spectral detector Pulsed and continuous lasers
OTHER	GPC <i>Waters</i>	Molecular weight, polydispersity	-	-	-	Analysis in different solvents and columns
	LS <i>Wyatt Dawn eos - qels - optilab</i>	Molecular weight, R _g , R _h , second virial coefficient (A ₂), dn/dc	-	-	-	Multi-angle detector Static and dynamic light scattering
	Elemental analysis <i>Fisons SPA EA1108; Costech 4010</i>	Quantitative analysis of C, H, N and S	0.3%	-	-	
High-throughput synthesis and purification						
	Techniques / Instruments	Characteristics			Applications	
HIGH THROUGHPUT SYNTHESIS	Microwave-assisted synthesis <i>Biotage, Initiator with robot-60 CEM MARS-X and MARS-5</i>	Programmable and robotized, T = 50 - 250 °C and P = 1 - 17 bars Fast and efficient air cooling of reaction vessels Up to 14 or 40 samples run simultaneously			Method development and sample preparation Reaction scale from 0.2 mL to 20 mL Reaction volumes from 5 to 100 mL	
	Multiple robotic stations <i>Mettler-AutoChem Robotic</i>	Weighing, reagent-dispensing, and liquid-liquid extraction stations Multiple reaction blocks for 6, 12, 24 tubes, inert atmosphere, heating, cooling, magnetic stirring and shaking			Method development Production of chemical libraries	
	Evaporative vacuum centrifuges <i>Genevac Model HT4X (2 units)</i>	4 position holders, IR-heater compensator, -70°C cooling chamber, handles tubes and plates			Isolation of crude product after reaction or work-up	
	Lyophilizer <i>Virtis Model FM25EL</i>	12-port system, multiple glass bottles available Evaporates aqueous/acidic/basic solutions			Isolation of products following HPLC purification	
ANALYSIS AND PURIFICATION	Analytical HPLC (DAD) <i>Waters Alliance</i>	MasLynx software, open-access system, multiple column operation			Analysis of reaction mixtures and products Analytical tool required for method development	
	Supercritical fluid chromatography <i>4 analytical Thar-Berger systems 1 preparative-70 Thar system</i>	UV detection, auto column switching, Gilson fraction collection, numerous chiral columns			Optical purity determination (<i>ee</i> , <i>de</i>) Separation/isolation of stereoisomers	
	Flash chromatography <i>Biotage SP4 systems (4 units)</i>	Manually activated, UV-directed fraction collection, 3 different column sizes, gradient elution			Purification of compounds	