

## Center Macromolecular Structure Analysis: Equipment

### Optical spectroscopy

#### FTIR spectrometer Vertex 70 (Bruker)

- DTGS and MCT detector
- accessories for reflection methods: ATR (also temperature-dependent), DRIFT, IRRAS (also heatable)
- variable temperature cell (SPECAC) for temperature-dependent measurements from RT up to 700 °C
- connected FTIR microscope (HYPERION) with XY-cross table as well as programmable microscope hot stage and motorized knife edge aperture
- automatic search of spectra with different commercial-available and self-made data base libraries
- micro flow cell (AABSPEC mode #RA4000-EXP) for coupling of SEC/FTIR
- rheo-optical extension, rapid scan-mode

#### FTIR spectrometer Vertex 80v (Bruker)

- DTGS and MTC detector
- IRRAS (also heatable)
- external sample compartment: "Golden Gate Diamant ATR" (SPECAC) also temperature-dependent up to 200 °C
- integration module (Ulbricht sphere) for NIR with sample rotator for inhomogeneous samples

#### AFM-IR NanoIR 2 (Anasys/Bruker)

- OPO laser (3600-900 cm<sup>-1</sup>)
- contact mode

#### FT-IR Imaging system Spotlight 400 (PerkinElmer)

- microscope detector: MCT line detector (imaging) and MCT single detector
- spectrometer detector: LiTaO<sub>3</sub> MIR detector
- operating modes: single spectra/ spectral imaging in transmission and reflection, micro-ATR
- particle recognition software

#### RAMAN microscope alpha 300R+ (WITec)

- 532 nm and 785 nm laser, UHTS 300 spectrometer, EMCCD detector, heatable microscope stage,
- External fiber-coupled probe for in-situ measurements
- operating modes: single spectra, times series, spectral 2D/3D imaging, depth profiling, True Surface (topographic profiling), bright field and dark field, resolution: 240 nm laterally
- external particle recognition software GEPARD

#### RAMAN microscope inVia Qontor (Renishaw)

- 532 nm, 633 nm and 785 nm laser, detector: CCD
- operating modes: single spectra, surface montage, spectral 2D/3D imaging, Live Track™, Focus Track™, bright field and dark field, resolution: 240 nm laterally
- Internal and external particle recognition software

#### Particle software GEPARD

- for optical, FTIR- and Raman microscopes (Open Source software)

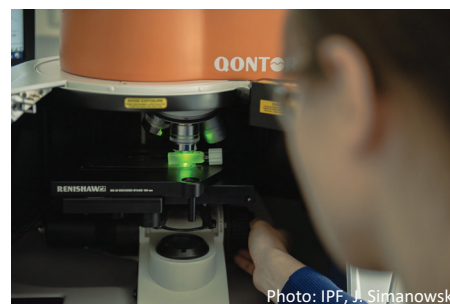


Photo: IPF, J. Simanowski

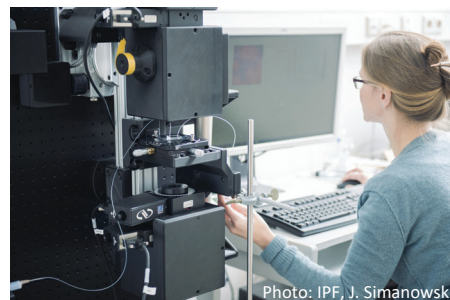


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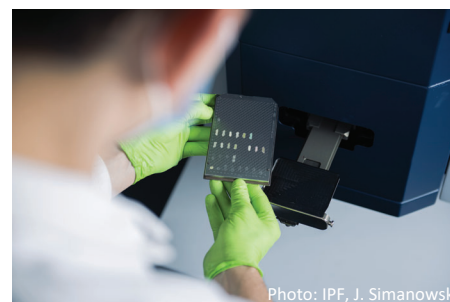


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## Chromatography, fractionation und light scattering

### Asymmetrical flow-field flow fractionation (AF4)

- Eclipse 3 (Wyatt Technologies Corp., USA), organic/aqueous, with isocratic pump, autosampler, UV and RI detector, and DAWN EOS MALS detector (18 angles, Wyatt Technologies Corp., USA)
- Eclipse Dualtec (Wyatt Technologies Corp., USA), aqueous, with isocratic pump, autosampler, UV and T-rEX-RI-detector, and HELEOS II MALS detector (18 angles, with QELS-module), Thermo Pro temperature control unit (Wyatt Technologies Corp., USA)

### Thermal field flow fractionation (ThFFF)

- Complete system TF2000 (Postnova) with RI and MALS detector (Postnova Analytix GmbH, DE)

### Size exclusion chromatography (SEC)

- different organic solvents (ambient and high temperature) and aqueous eluent (RT)
- Isocratic pumps, DA-, viscosity and RI detectors as well as autosamplers of 1100 and 1200 series (Agilent Technologies)
- Optilab T-rEX RI detector, TREOS and HELEOS II MALS detectors, QELS modules, Viscostar III (Wyatt Technologies Corp. USA)

### Gas chromatography (GC)

- pyrolysis GC MS: pyroprobe (CDS Analytical Inc.) and GC7890A as well as MSD 5975C (Agilent Technologies)
- Headspace-GC-MS: Headspace sampler 7694, GC6890N and MSD 5973N (Agilent Technologies)

### Batch characterization

- dynamic light scattering: DynaPro Nanostar (90°) from Wyatt Technologies Corp.
- Zeta potential measurements and dynamic light scattering: Zetasizer Nano Z (0-90 °C) with MPT-2 autotitrator (Malvern, UK)
- Microviscometer; Lovis (20-90 °C) (Anton Paar GmbH, Austria)

## MALDI-TOF-MS

### Autoflex Speed TOF/TOF System (Bruker)

- LC/MALDI-TOF-MS spray deposition interface ESAirD (BAM, Germany)

## Elemental analysis

### Elemental analyzer vario MICRO cube (Elementar)

- Determination of H, C, N and S content

## NMR spectroscopy

### NMR spectrometer Avance III 500 (Bruker)

- 3 HF channels (X;  $^1\text{H}/^{19}\text{F}$ ; Y)
- z gradient accessories, temperature control unit and autosampler
- QNP probe ( $^1\text{H}$ ;  $^{13}\text{C}$ ;  $^{19}\text{F}$ ;  $^{31}\text{P}$ ) with z gradient
- TBI probe ( $^1\text{H}$ ;  $^{13}\text{C}$ ;  $^{31}\text{P}$ - $^{109}\text{Ag}$ ) with z gradient
- BBO probe ( $^1\text{H}$ ;  $^{19}\text{F}$ ;  $^{31}\text{P}$ - $^{109}\text{Ag}$ ) with z gradient
- 10 mm triple resonance probe ( $^1\text{H}$ ; X;  $^{31}\text{P}$ )
- 4 mm HRMAS probe ( $^1\text{H}$ ;  $^{13}\text{C}$ ) with z gradient

## Optical characterization of thin films

### Rotating compensator multi wavelength ellipsometer alpha-SE (J.A. Woollam Co. Inc.)

- spectral range 380-900 nm, incidence angle 65°, 70° and 75°, with temperature and/or pH controlled in-situ fluid cell

### Rotating compensator multi wavelength ellipsometer M2000 UI (J.A. Woollam Co. Inc)

- spectral range 245-1700 nm
- incidence angle 45°-90°

### Digital Multiple Wavelength Refractometer DSR Lambda (Schmidt + Haensch GmbH & Co.)

### Müller matrix microscope (ACOM, University Nebraska-Lincoln)

- two rotating compensators,
- spectral range 250-1000 nm,
- single wavelength measurement modus, combinable with optically transparent microfluidic cells

### Quartz crystal microbalance (Qsense, Biolin Scientific, Sweden)

- combinable with spectroscopic ellipsometry (alpha-SE, M2000 UI) or electrochemistry module

## Thermal analysis

### Thermobalance Q 5000 (TA Instruments)

- 40 up to 1000 °C, with autosampler, nitrogen or air, optionally coupled to FTIR spectrometer Nicolet 380 (Thermo Electron) and to GC-MS (Agilent) via IST16 interface (SRA Instruments)

### Dynamic differential calorimeter DSC Q 1000 (TA Instruments)

- -80 up to 400 °C, with autosampler, nitrogen, optionally temperature-modulated

### Dynamic differential calorimeter Discovery DSC 2500 (TA Instruments)

- -120 up to 400 °C, with autosampler, nitrogen and air, optionally temperature-modulated, with RCS120 cooling system

## Contact

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