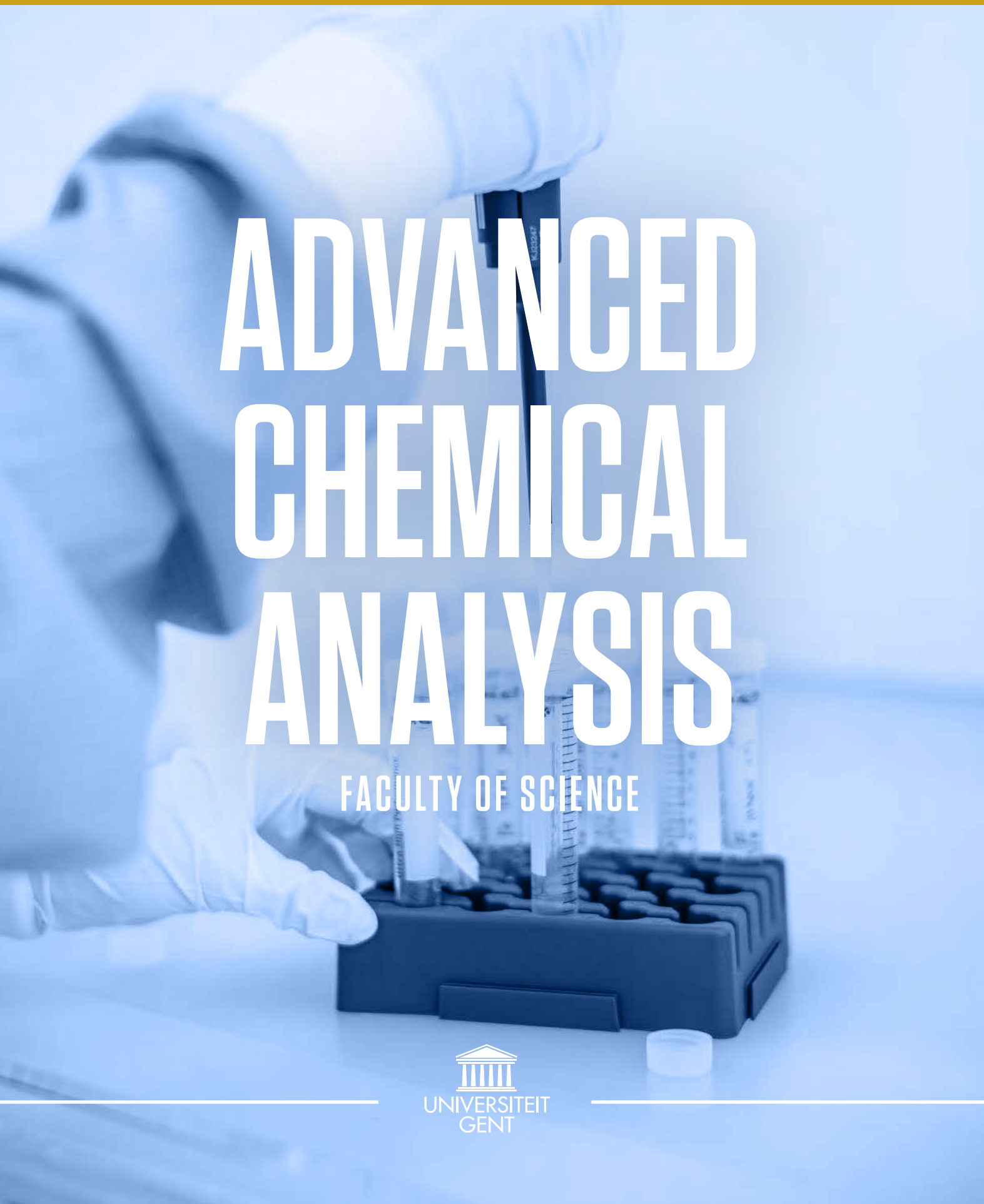
EXPERTISE AT UGENT



ADVANCED CHEMICAL ANALYSIS

FACULTY OF SCIENCE

UNIVERSITEIT GENT

OUR OFFER

SOLUTIONS BASED ON ADVANCED STRUCTURAL AND ANALYTICAL TECHNOLOGIES

Business Focus: Advanced Chemical Analysis offers **specialized, powerful and robust integrated or combined structural and analytical solutions** to support the Pharma, Food, Chemical & Polymer industries. Through its collaborations, this analysis platform provides access to a unique combination of applied analytical science expertise, with **state-of-the-art technology and innovative approaches** based on technologies such as advanced NMR methods, chromatographic technologies, Atomic and mass spectrometry, X-ray crystallography (XRD) techniques and Vibrational Optical Activity methods.

We provide our clients with a **toolbox of technologies and knowledge** to support and strengthen their Research, Development and Quality Analysis activities related to the following 4 categories. We offer solutions to challenges in:

PURITY & CONTAMINANTS

Detection and quantification of organic and inorganic impurities in a wide range of substrates. Targeted determination of contaminants on the surface of objects.

PROFILING & FINGERPRINTING

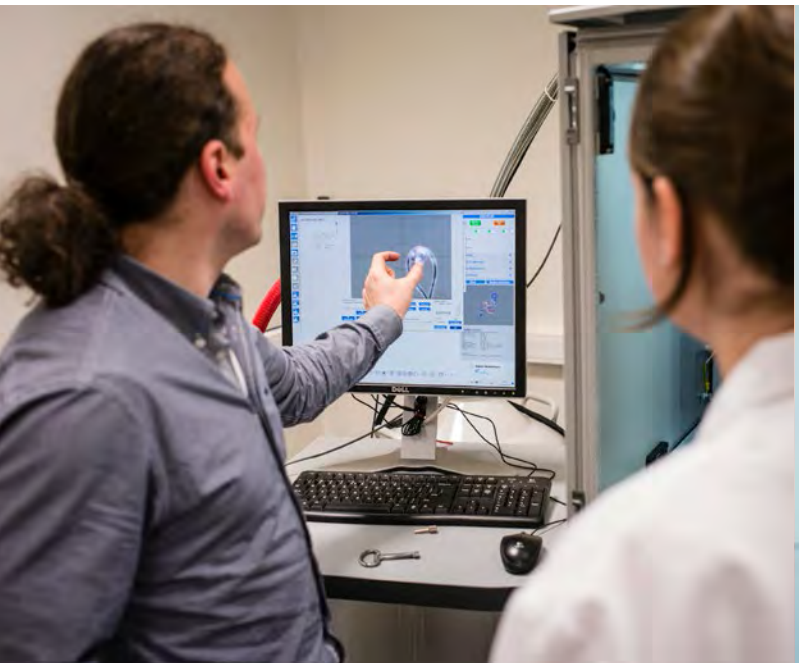
Chromatographic profiling as a tool in the comparison and evaluation of complex mixtures. Use of multivariate analysis for screening and quantifying the contributions of individual components. Improve the link from analytical data to information.

DISTRIBUTION & SPATIAL MAPPING

Analytical tools for creating a visual image of the variation in the chemical composition by measurement of spectra and spatial - time information.

STRUCTURE & INTERACTION

Determination of structure and absolute configuration of molecules. Tools for studying the interaction and conformational changes of small and large molecules.



OUR OFFER

PURITY & CONTAMINANTS

STRUCTURE & INTERACTIONS

PROFILING & FINGER-PRINTING

DISTRIBUTION & SPACIAL MAPPING

OUR TOOLBOX

Solutions are based on innovative approaches and state-of-the-art technology or combinations of technologies such as advanced NMR methods, chromatographic technologies including advanced GC, LC, electrophoresis CEC, SFC, Atomic and mass spectrometry based on ICP-MS and ICP-OES, elemental speciation using the coupling of HPLC and ICP-MS, Isotopic analysis using TIMS or multi collector ICP-MS, bulk and spatially resolved elemental analysis of solid samples via the coupling of laser ablation (LA) and ICP-MS, X-ray crystallography (XRD) techniques and Vibrational Optical Activity methods, including Vibrational Circular Dichroism (VCD) and Raman Optical Activity (ROA).

High performance Chromatography
Use of Advanced separation techniques such as Gas Chromatography (GC), Liquid Chromatography (HPLC, LC) , Capillary Electrophoresis & Capillary Electrochromatography (EP & CEC), Supercritical Fluid Chromatography (SFC). With focus on hyphenation techniques; i.e. coupling the separation techniques to state-of-the-art spectroscopic detectors, such as MS detectors and NMR. e.g. – column and stationary phase development, comprehensive (LCxLC) system development, pre-concentration phases for femtogram analysis, method developement and modeling.

X-Ray crystallography
Use of Single Crystal X-Ray Diffraction (XRD), (crystallization + X-ray structure determination), for crystallographic services for: small (in)(metal-)organic molecules, metal-organic frameworks (MOFs), determination of the absolute configuration.

Vibrational Optical Activity methods
Analytical service centre providing a knowledge based service for applications requiring structural elucidation of chiral molecules using techniques as Vibrational Circular Discroism (VCD) and Raman Optical Activity (ROA), collectively known as Vibrational Optical Activity (VOA). Importantly no crystallization is required as measurements are performed in solution.

NMR spectroscopy
NMR method development in 1H NMR, 13C APT, 2D COSY, TOCSY, ROESY, NOESY, HSQC, HMBC and combinations thereof. e.g. solution NMR methods for colloidal quantumdots, Diffusion NMR spectroscopy and hr-MAS NMR, Rapid TOCSY typing of complex carbohyrbrates.

Atomic and mass spectroscopy
Method development for trace element analysis using quadrupole-based ICP-MS instruments equipped with a multipole collision/reaction cell, high-resolution sector-field ICP-MS or tandem ICP-MS. High-precision isotopic analysis using multi-collector ICP-MS. Elemental speciation using HPLC-ICP-MS. Bulk and spatially resolved analysis (including mapping and depth profiling analysis) of solid materials using LA-ICP-MS.

OUR EXPERT TEAM

PROF. JOSÉ MARTINS
NMR Structure Analysis Unit

PROF. FRANK VANHAECKE
Atomic & Mass spectrometry Research Group

PROF. KRISTOF VAN HECKE
X-Struct research group

PROF. PATRICK BULTINCK
Quantum Chemistry Research Group

PROF. FREDERIC LYNEN
Separation Science Group

The **Separation Science Group** is studying the underlying phenomena controlling physical separation in chromatography, electrophoresis, filtration and mass spectroscopy. Research interest ranges from innovative column technology, the development of entirely new separation systems, the quest for ever higher separation efficiencies in less time, green chromatography, high recovery sample preparation approaches, improved preparative analysis, improving sensitivity and linear range limits of quantitative approaches and ever better hyphenation with spectroscopic techniques.
The more applied research components involve high-end applications of state-of-the-art technology to address core issues in life sciences, pharmaceutical, fine, organic and polymer chemistry industry sectors.

The **NMR Structure Analysis Unit** is focusing on Nuclear Magnetic Resonance spectroscopy. The team's expertise ranges from structure elucidation and conformational analysis of natural or synthetic bioactive compounds, over method development for the investigation of colloidal dispersions of semi conductor nanocrystal or organic pigments, to host-guest interactions in supramolecular chemistry, biomolecular NMR or the analysis of metabolites in biological fluids such as blood serum or cerebrospinal fluid. The group hosts the high field 700 MHz interuniversitary NMR facility. This unique technological platform is open to researchers from academic institutes as well as industry.

The **Atomic & Mass spectrometry research group** is specialized in the determination, speciation and isotopic analysis of (trace) elements using ICP-MS. The research group has state-of–the-art ICP-MS instruments at its disposal. Three quadrupole-based ICP-MS equipped with a collision/reaction cell; an ICP-MS/MS unit equipped with an octopole collision/reaction cell; a single-collector sector field ICP-MS that can be operated at higher mass resolution; and a multi-collector ICP-MS as a dedicated tool for high-precision isotopic analysis. The team has expertise with a variety of sample introduction techniques, including miniaturized nebulizers, aerosol desolvation units, laser ablation systems and chromatographic separation techniques.

The **X-Struct research group** focuses on using X-ray diffraction for structure elucidation in general and more specifically in the field of Bio-Inorganic Chemistry. Single crystal X-ray diffraction (XRD) or crystallography is by far the most accurate way to obtain 3D structures of molecules at the atomic level. The team uses this technique to determine the molecular structures of several compounds, ranging from small (in)organic molecules, ionic liquids (IL's), metal-organic complexes and frameworks (MOF's), bio-inorganic materials to modified DNA oligonucleotides and peptides.

The **Quantum Chemistry Research Group** focuses on (computational) quantum chemistry, with emphasis on framing classical chemical concepts in quantum mechanics, quantitative structure-activity relationships, vibrational circular dichroism experiment and modeling and programming as a major part of all the above topics.

CONTACT INFORMATION

The Advanced Chemical Analysis cluster is supported by the business unit **ChemTech**, that aims to be the focal point for **industrial collaborations** between research groups dealing with chemistry and companies that are looking for chemical expertise.

ChemTech facilitates and coordinates a set of **industrial projects** and manages a **strategic IP portfolio** and its licensing opportunities.

The business developers of ChemTech are at your disposal:

DR. AN VAN DEN BULCKE
ChemTech Technologies
for Lifesciences

Krijgslaan 281, S4
B–9000 Gent – Belgium
A.Vandenbulcke@UGent.be
www.chemtech.ugent.be
T +32 9 264 44 62
M +32 474 81 23 81

DR. BART HOMMEZ
ChemTech Technologies for
Material and Chemical Industries

Krijgslaan 281, S4
B–9000 Gent – Belgium
Bart.Hommez@UGent.be
www.chemtech.ugent.be
T +32 9 264 96 03
M +32 471 99 41 94

AC2015/05-v2