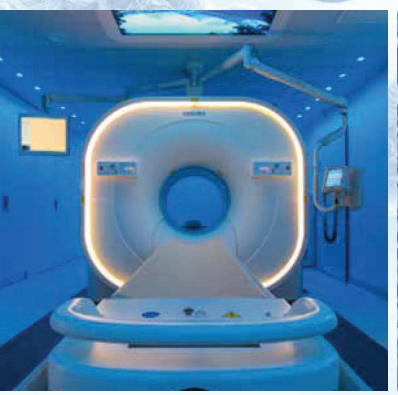
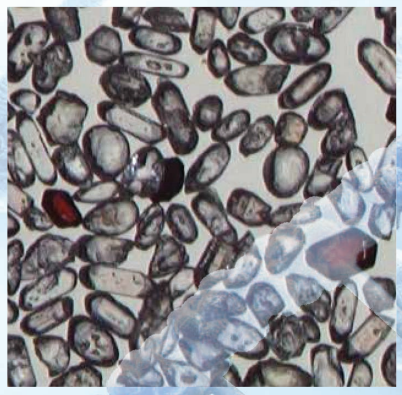
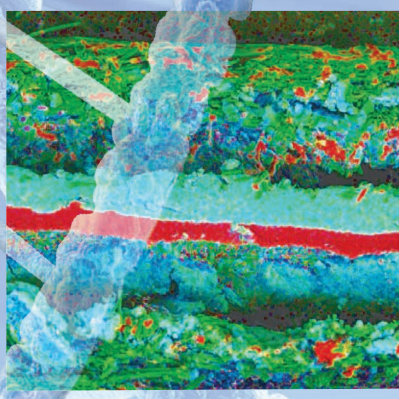
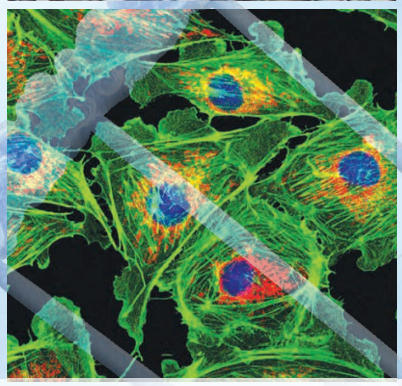
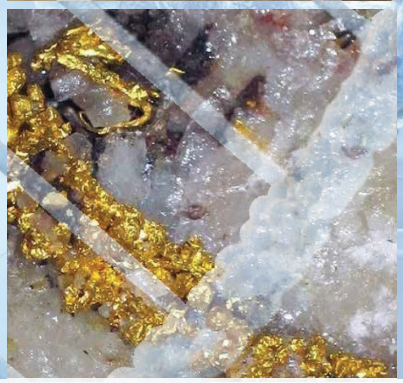
CAF Central Analytical Facilities
STELLENBOSCH UNIVERSITY

2018/2019 Annual Report of the Central Analytical Facilities

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Ms Fransien Kamper
Dr Alex Doruyter

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Overview

The Central Analytical Facilities (CAF) at Stellenbosch University (SU) has become a *de facto* national facility in South Africa. This is evidenced by the fact that during 2018, income derived from analytical services was split almost equally between SU clients, clients from other South African universities, and industry clients.

As the range of analytical services offered by CAF continues to grow, it is predictable that the proportion of income derived from Stellenbosch University will continue to decrease, while the amount of work conducted for SU clients will continue to grow. This is good for our university, as it makes our analytical services more affordable, brings collaborative work to Stellenbosch and makes our institution attractive to the postgraduates studying elsewhere who rely on our analytical services. It also demonstrates that we do indeed meet our mandate to build capacity and to transform the profile of South Africans with higher degrees; even including a sizable community of post-graduate students who are not registered at our institution.

During 2018, 308 PhD and MSc students from other South African universities used CAF services; for the first half of 2019 this figure is 176. Thus, the exceptional array of expertise and large equipment infrastructure within CAF is helping to facilitate research and educate people at many South African institutions. It is important to note that this level of impact would not be possible without the investment in large equipment by SU and the National Research Foundation, through the National Equipment Programme (NEP). It is truly a privilege for all CAF staff members to be in a position to play such a profoundly important role in capacity building within South Africa.

As can be seen in the graph (on the right), the NEP has been and still is critically important for creating and maintaining analytical capacity within CAF. However, in 2016 the Department of Science and Technology launched the South African Research Infrastructure Roadmap (SARIR), which has changed the landscape for large equipment funding to a significant degree, with competitive NEP funding rounds now occurring only every second year. This programme will create extensive and complex research infrastructure often spanning several institutions to address national needs.

CAF is involved with two SARIR infrastructure projects. The first is the Nuclear Medicine Research Infrastructure Platform (NuMeRI) and the second is the Biogeochemistry Research Infrastructure Platform (BIOGRIP). The NuMeRI Node for Infection Imaging will be launched at Tygerberg Hospital in November 2019 and the BIOGRIP Node for Water and Soil Analysis will hopefully be inaugurated by early 2020 at the latest. Both these platform nodes will be managed as financially ring-fenced structures within CAF, and the work that will be conducted within the NII is detailed within an article in this report.

As CAF strives to stimulate research by keeping costs to academic clients as low as possible, there is always some risk in any given year that CAF income will fall below costs. As indicated in the graph (on the right), this is likely to occur in 2019, for the first time in several years, with a projected deficit of R682 637. This has occurred as a result of declining income over 2018 values at several CAF units, principally CT Scanner (CT), Electron Microscopy (EM) and Fluorescence Microscopy. (FM). This has been compounded by unusually large equipment repair bills at the CT and ICP-MS units. CAF will recover this deficit in 2020 through new services built around the three new NEP-funded large equipment items acquired in 2019, the Amnis Imaging Flow Cytometer, the Mass-Directed Auto Purification system, and the Gemini 300FE SEM with advanced 3D imaging. The inauguration of the two SARIR nodes managed by CAF will also have a positive influence on demand for specific synergistic services within established CAF units.

Prof Gary Stevens
CAF Director

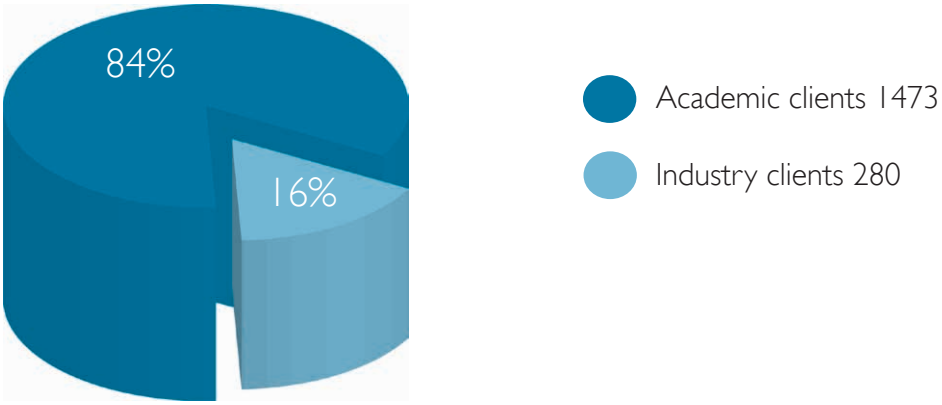
CAF income and costs over the past five years and a projection for 2019 with NEP equipment acquisitions and surplus/deficit as percentage of income.

Combined value of the NEP acquisitions | Income | Costs | Surplus/Deficit

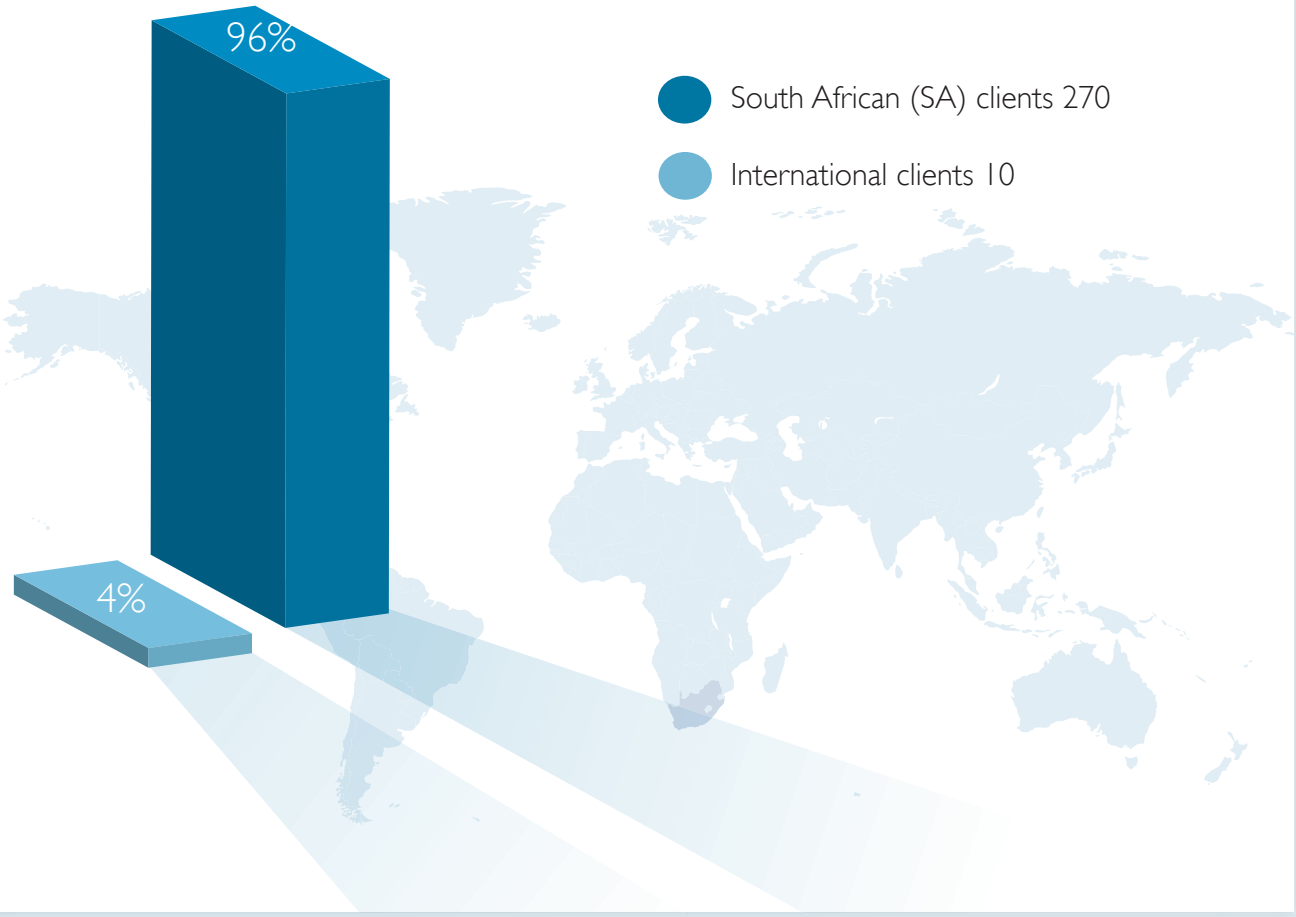
Profile of CAF clients

Since 2017, all CAF clients have had to register online before they could use equipment in a CAF laboratory. This enables CAF to provide the NRF with a comprehensive profile of the use of NEP-funded equipment. The following graphs provide some information on the CAF client profile in 2018:

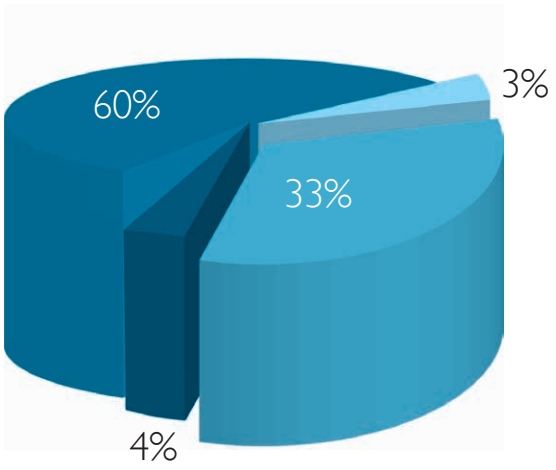
The proportion of CAF academic clients relative to industry clients:



The proportion of local industry clients relative to international industry clients:

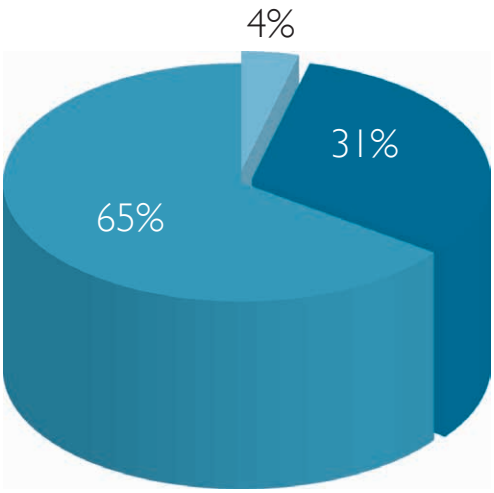


The proportions of different kinds of academic clients:



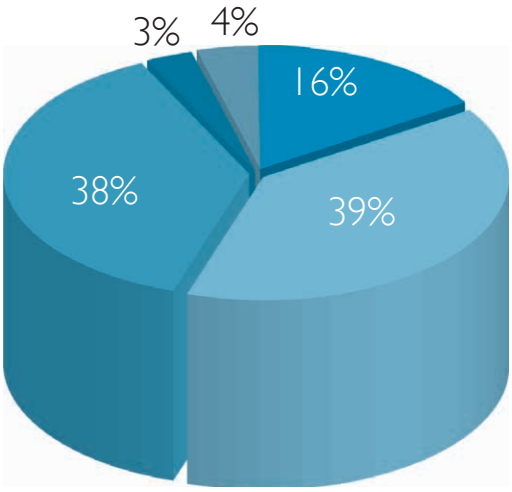
- Other SA universities 480
- SA Research Institutions 65
- Stellenbosch University 878
- International universities 50

The profile of CAF academic clients:



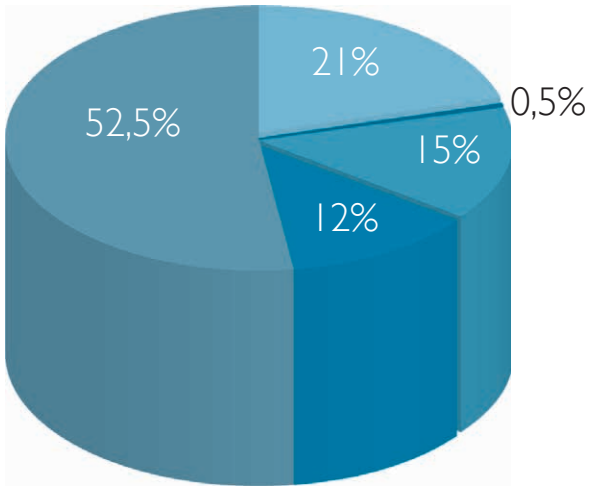
- Research assistants 59
- Researchers 455
- Students and Post-Doctoral fellows 959

The subdivision of the 65% students and post-doctoral fellows from the previous graph:



- Honours 150
- Master's 377
- PhD 364
- Postdoc 31
- Undergraduate 37

The proportions of Stellenbosch University student clients according to faculty:



- AgriSciences 134
- Education 2
- Engineering 95
- Medicine and Health Sciences 81
- Science 339

Digital, time-of-flight **molecular imaging**

By Alex Doruyter

Positron Emission Tomography, combined with (x-ray) Computed Tomography (PET-CT), has revolutionised the field of nuclear medicine. Using PET-CT makes it possible to non-invasively visualise, quantify, and localise diverse biological processes in health and disease with a high degree of accuracy. The Node for Infection Imaging (NII), a new analytical structure managed by CAF, with state-of-the-art PET-CT facilities, is scheduled to start operations in November 2019 and promises to become a powerful tool for researchers in infectious disease and other medical fields.

Introduction

Nuclear imaging exploits a fundamental property of certain unstable atoms, namely that they will undergo radioactive decay by either directly or indirectly emitting gamma photons. A mode of decay in which an unstable nucleus ejects a positron results in a matter-antimatter (annihilation) reaction when this positron meets a neighbouring electron. During annihilation, the combined mass of the particle-antiparticle pair is converted into energy, in the form of two 511 keV gamma photons travelling in opposite directions (Fig 1).

By labelling biological molecules of interest with positron-emitting radionuclides it becomes possible, using specialised equipment, to image the approximate position of annihilation events and hence, the three-dimensional location of the molecule in question. This imaging is performed with a positron-emission tomography (PET) scanner (Fig 2), which is routinely combined with a conventional (x-ray) computed tomography (CT) system in modern scanners. The combined ability of such PET-CT systems to quantitatively and dynamically image the behaviour of radiolabelled molecules of interest (radiotracers) with a high degree of accuracy, and to localise their distribution precisely with the anatomical definition provided by their CT component, has revolutionised biological research.

Possibilities

The diversity of physiological and pathological processes that can be studied with PET-CT is vast. They include various forms of energy metabolism (e.g. glucose, amino acid, fatty acid); neurotransmitter function (e.g. dopamine, serotonin, opiate); receptor or enzyme expression (e.g. somatostatin, prostate-specific membrane antigen); organ perfusion; ischaemia; antibody function and more.

Amenable processes that may be studied with PET-radiopharmaceuticals are limited only by the chemistry involved in producing the necessary tracer molecule; the availability and half-life of the radionuclides used to label them; and radiation exposure constraints. Examples of PET-CT scans using different radiotracers appear in Fig 3-6.

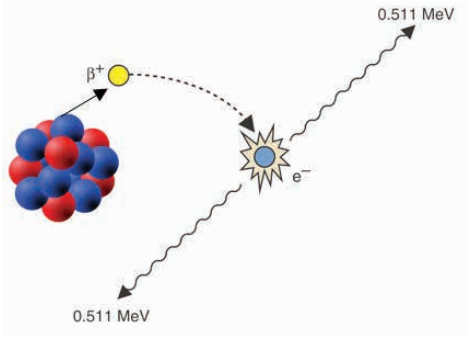


Figure 1: Positron emission with annihilation event. After ejection from an unstable nucleus, a positron combines with a nearby electron and undergoes annihilation. The resultant 511 keV gamma photons travel at 180° to one another.

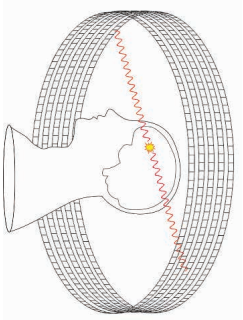


Figure 2: Positron Emission Tomography. A circular array of specialised detectors registers the arrival of coincident gamma photons. Multiple intersecting "lines of response" allow accurate 3D localisation of local concentrations of radiotracer.

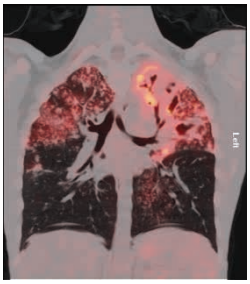


Figure 3: Limited-field PET (using F-18 FDG) fused with serially acquired CT in a patient with tuberculosis. Intensity of uptake on the PET correlates with metabolic activity within lesions.

PET research at SU

Stellenbosch University (SU) researchers have been conducting PET-CT research since 2011, when scanning was still performed on a private PET-CT camera at Panorama Hospital. Since the establishment of the Western Cape Academic PET-CT Centre (WCAPC) at Tygerberg Hospital in March 2012, researcher demand for PET-CT scans has grown rapidly.

To date, most research studies at WCAPC have been performed to assess metabolic activity of tuberculosis (TB) lesions using a glucose tracer, fluorine-18 fluorodeoxyglucose (F-18 FDG). This work has, for example, made important contributions to understanding the biological significance of persistent Mycobacterium tuberculosis mitochondrial RNA (mRNA) in TB patients after completing therapy;[1] and in evaluating mRNA and other potential TB biomarkers.[2,3] It has also led to new methods in quantifying pulmonary disease burden;[4] as well as shown value in identifying HIV patients with latent TB at risk for disease progression.[5] FDG PET-CT research is ongoing in contacts of patients with multidrug resistant TB (to identify early disease); in patients with active pulmonary TB (to map disease activity during therapy); and in patients with spinal TB (to determine optimal therapy duration).

Several different types of cancer, such as lung cancer, lymphoma and cervix cancer, avidly accumulate FDG, and PET-CT has an important clinical role in the management of many malignancies.[6,7] Several SU research projects investigating the role of PET-CT in staging and measuring treatment response in these cancers have been published,[8–10] or are still in progress.

FDG is also an excellent proxy marker for neural activity in the brain, and SU researchers have used it for investigating the neurobiology of social anxiety disorder;[11] and the brain effects of methamphetamine abuse.[12] Projects investigating the neural basis of functional tremor; optimising brain PET reconstruction; and establishing a local normal FDG brain database, are currently underway.

While most PET-CT research performed by SU has focused on glucose metabolism (using F-18 FDG), other projects using a somatostatin-receptor binding compound (the somatostatin analogue Gallium-68 DOTANOC) to image neuroendocrine tumours; and a prostate cancer binding agent (Gallium-68 PSMA) are ongoing.[13,14] Provisional results of research using F-18 FDOPA PET-CT, a proxy means of evaluating presynaptic dopaminergic function in patients with movement disorders, have been presented at an international congress.[15]

PET research at SU has also focused on improvements in PET quantification, with current projects directed at optimisation of PET acquisition and reconstruction protocols, and the simulation of compartmental analysis of F-18 fallypride imaging. This work is ongoing in collaboration with the University of Freiburg (Germany) and KU Leuven (Belgium). SU radiopharmacy researchers have developed and optimised new kit formulations for Ga-68 DOTA compounds;[16,17] and have presented work on Ga-68 labelling experience internationally.[18] Projects on the automated synthesis of Ga-68 ubiquicidin (a candidate infection tracer) and on F-18 fallypride synthesis (used for post-synaptic dopaminergic neuron imaging) are underway.

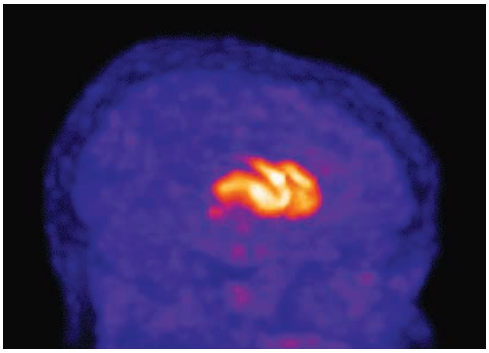


Figure 4: Anterior oblique projection of an F-18 FDOPA PET scan showing normal presynaptic dopaminergic function in bilateral striatal structures of the brain.

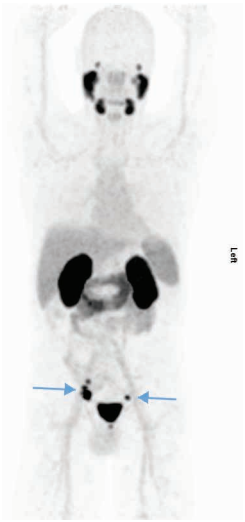


Figure 5: Whole-body projection of a PET scan performed using Ga-68 prostate-specific membrane antigen (PSMA). In addition to normal biodistribution, spread of prostate cancer to multiple lymph nodes (arrows) is visible.

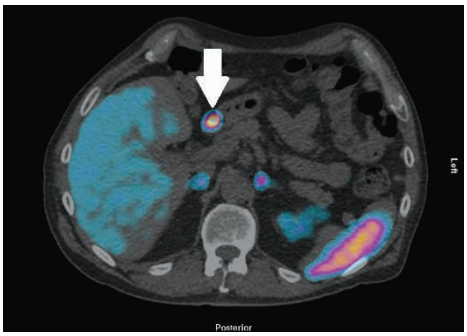


Figure 6: PET images acquired using Ga-68 DOTANOC (a somatostatin analogue) fused with serially acquired CT, of a patient suspected of having a neuroendocrine tumour of the small bowel. This tumour (arrow) was undetectable on anatomical imaging or on endoscopy but was confirmed by histology.

The Node for Infection Imaging

In 2014, the scientific nuclear medicine community prepared a proposal for the South African Research Infrastructure Roadmap (SARIR). This national roadmap was developed to prioritise the establishment of core national research infrastructure for the benefit of the local and global scientific community.

The Nuclear Medicine Research Infrastructure Project (NuMeRI) was one of seven projects selected for initial rollout. It was within the NuMeRI structure that the Node for Infection Imaging (NII) was conceived. The NII is a new, dedicated PET-CT research facility currently (2019) under construction on the grounds of Tygerberg Hospital (Fig 7), which will be managed as a NuMeRI Node by the Central Analytical Facilities of SU. The facility has procured a top-of-the-line, time-of-flight, digital PET-CT scanner (Fig 8), which promises to ensure high-quality research imaging with lower doses of radiation. In addition, recognising the need for more advanced radiotracer research, an important component of the NII project is the installation of an expanded radiopharmacy, with all necessary equipment to perform more advanced labelling procedures and to develop novel tracers. Although the NII will largely focus on research in infectious diseases (mainly TB), the state-of-the-art facilities are expected to benefit a wide range of clinical and basic science researchers. The NII is projected to commence operations early in November of 2019.

Figure 7: Construction of the NII adjacent to the Western Cape Academic PET-CT Centre.

Figure 8: The Philips Vereos PET-CT system.
Image credit: www.Philips.com

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Biomedical
Mass Spectrometry Division

By Hannes van der Merwe, Maré Vlok and Marietjie Stander

Research involving human samples has always been under scrutiny by regulators to ensure that the data generated is accurate and reliable, to ensure the safety of patients and trial subjects, as well as ensuring that the analyses performed at different facilities are comparable and research involving humans is performed in an ethical manner.

The regulation and guidance documents governing research involving human samples are regularly updated to ensure that they remain up to date with the latest technologies, industry trends and an ever-changing regulatory environment with the intent to minimise risk, error and fraud. Laboratories operating in these environments face different challenges than those operating in a more traditional environment, as incorrect data can lead to life-threatening results as well as damage to the reputation of both the client and the laboratory.

The CAF Biomedical Facility at Tygerberg was born out of the need to have analytical services available in close proximity to clinical researchers, the medical faculty and the research hospital.

CAF already had a number of units in operation at Tygerberg and the incorporation of the LC-MS and HPLC facilities in the Pharmacology Department created the opportunity for close collaboration between the traditional small-molecule (<2kDa) laboratory, under the control of newly appointed Hannes van der Merwe and the Mass Spectrometry Proteomics laboratory of Maré Vlok. This new division of the MS Unit, which is managed by Dr Marietjie Stander, is known as the Biomedical Mass Spectroscopy Division. It can now consult as single entity and give clients the opportunity to conduct a more complete analysis of their sample, as well as investigating both the pharmacokinetics (PK) and pharmacodynamics (PD) in aspects of samples.

Small molecules (<2kDa):

Liquid chromatography-tandem mass spectrometry (LC-MS/MS) has become the standard in clinical laboratories for analysis of samples over the last few decades. It offers much higher specificity than that of immunoassays or conventional high-performance liquid chromatography (HPLC) for low molecular weight analytes. Traditional triple quad LC-MS apparatus is ideal for studying and monitoring compounds less than 2kDa in size. These include many therapeutic drugs, toxins and small biological molecules.

Figure 1: Tygerberg Medical Campus

Figure 2: Shimadzu 8040 LC-MS/MS.

The aim of the laboratory is to provide analytical services for academic researchers and industry clients in the fields concerned with medical devices or clinical trials. Methods are developed with the needs of the client in mind, and can range from basic validations to conforming to EMA and FDA requirements for submission purposes to medical registration bodies. The Biomedical Facility employs staff with a proven track record in the clinical laboratory industry and maintains a quality system for ensuring continuous improvement and keeping up to date with industry trends and requirements.

Biological samples are complex matrices, and therefore extraction methods are developed and optimised before analysis to minimise any matrix effects. These extraction methods are part of the services provided and can include solid-phase extraction (SPE), liquid-liquid extractions (LLE) and precipitation steps that are selected according to the project needs and budget, and optimised to ensure high extraction yields and repeatability. Applications of LC-MS range from food analysis and environmental testing to drug development work and medical device testing. LC-MS/MS allows for the development of highly selective methods to be applied on complex matrixes, yielding high-quality and repeatable results.

Proteomics

The Proteomics Facility is equipped with a state of the art mass spectrometer, a Fusion LTQ Orbitrap, which is the first of its kind in South Africa. It enables researchers with the opportunity to analyse thousands of proteins in one run. It also allows SA researchers the chance to compete with international proteomic researchers, albeit at a local price, without compromising the data quality. The laboratory also assists clients with identifying new biomarkers in clinical research with targeted and non-targeted analysis of samples.

Zebrafish

The Biomedical Mass Spectroscopy Division works in very close collaboration with the Department of Pharmacology. This collaboration has resulted in not only the setting up of the new LC-MS laboratory, but also in the successful proposal to create a new Zebrafish breeding facility to be housed in the Tygerberg Animal Unit and a new Zebrafish Research Unit to be situated in the Pharmacology Department, adjacent to the Biomedical Facility.

The use of zebrafish in research was established in the 1960s and has since become increasingly important. Many characteristics make zebra fish a valuable model for studying human genetics and diseases. These include that zebra fish are 1) genetically quite similar to humans and 70% of human genes are found in zebra fish; 2) the fish are easier to breed and maintain than rodents and other animal models; 3) the effects of drug treatments are easy to monitor; 4) large numbers of eggs and larvae can be produced on a daily basis, ensuring a ready supply of animals for research; and 5) it is easy to introduce treatments with embryos that are able to absorb chemicals that have been added to their water.

Zebra fish are becoming an increasingly popular choice of model for screening and disease study due to the fast turnaround times and readily available biological material.

Research involving zebra fish will always rely on LC-MS apparatus to monitor the PK compounds given as intervention in disease studies or included for screening and to monitor biomarkers associated with diseases and conditions.

Toxicology

In collaboration with Pharmacology, the Biomedical Mass Spectrometry Division also acquired a qualitative database that can be used to screen samples for the presence of more than 2300 compounds, which includes toxins, drugs of abuse and pesticides. This method will provide life-saving services, ensuring that patients get the correct treatment in cases of accidental or intentional exposure.

Figure 3: Danio rerio (Zebrafish).

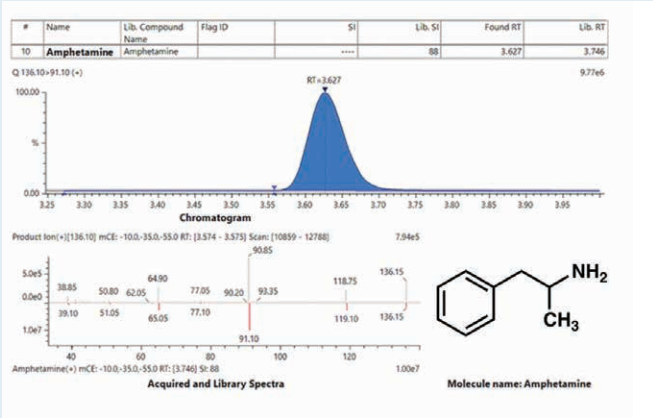


Figure 4: Result from the TOX-Screen database.

Future

The Biomedical Facility is relatively new, but as a result of some exciting new research projects, close collaboration with Pharmacology and the future developments on the Tygerberg Campus, we are looking forward to new opportunities and growth. The aim will remain to provide highly reliable analytical data while working according to the ISO15189 standard and the applicable GCP, GCLP and GLP guidelines as required by the project and client.

Figure 5: Future Biomedical Research Institute (BMRI) at the Tygerberg Campus.

Building a **sustainable** Nuclear Magnetic Resonance Facility

By Dr Jaco Brand and Dr Vincenzo Panebianco

The Nuclear Magnetic Resonance (NMR) Facility plays a critically important role in enabling high-quality chemistry research outputs and continuous hands-on post-graduate training. Over the years this facility has become largely self-sustainable. Several important components contributed to this accomplishment.

A diverse client base

According to 2017 and 2018 data, the facility had 188 academic and 25 industry users during this period. The academic users came from Stellenbosch University (SU) and 14 other South African universities, including previously disadvantaged institutions. As NMR is mostly a chemistry research tool, most of the unit's SU clients are academics, mainly from the Chemistry Department. An illustration of the post-graduate student utilisation of the facility during 2017 and 2018, according to the different categories of post graduate students, is presented in Figure 1.

The SU Chemistry Department published thirty-nine papers that relied on NMR data in 2018 alone. SU Chemistry had an impressive 13 PhD and nine MSc graduates that were also listed as regular NMR users during 2018; proof that this facility plays a pivotal role in supporting SU research output in the Faculty of Science in general, and in particular the Chemistry Department.

Using instrument time effectively

Although national academic clients forms the bulk of the facility's users, various industry clients also spend a significant amount of time on the instruments[1]. During the 2016 - 2018 period, a total of 7 227 hours were utilised in serving industry needs.

During the same three-year period, external academic users spent 10 373 hours and SU academics 64 039 hours of analytical time on the instruments. Overall, this translates into an average of 77% utilisation of the NMR instruments in support of academic research.

A sound base of industry clients

The NMR facility has grown to fund at least half of its expenses from its income and this has allowed the facility to operate very close to cost-effectively in most years with all operational costs, including salaries, covered by income (see Table 1).

Innovative administration

Having an effective administrative system saves a lot of time and ensures accurate monthly billing. Safety, security and operational awareness are maintained on a high level which ensures minimal breakdowns and downtime for repairs. Due to the specialised nature of the equipment, training is supplied continuously on an individual requirement basis. The facility also provides an annual hands-on training workshop to a selected group, which includes theory, interpretation and a

1 300, 400 and 600 MHz Agilent NMR spectrometers including a 500 MHz Solid State NMR spectrometer and a Circular Dichroism Spectropolarimeter

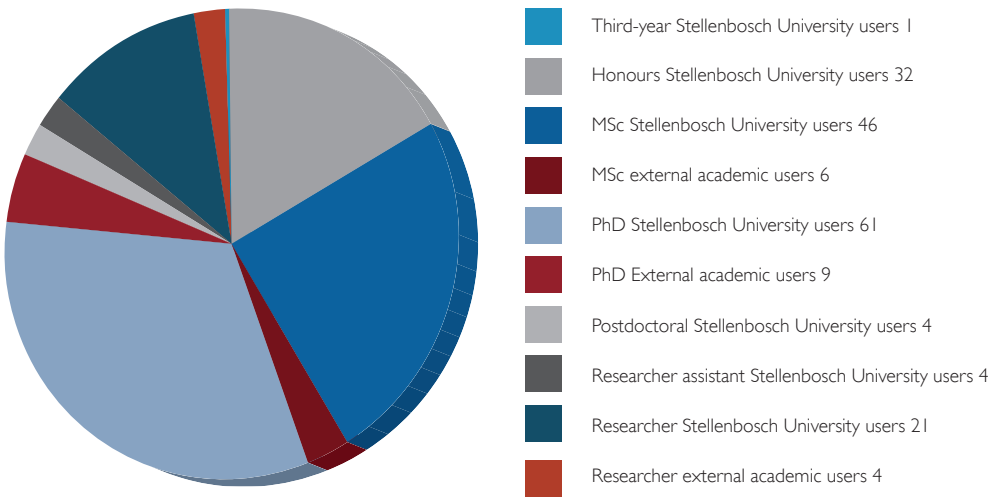


Figure 1: A spread of the clients utilisation of the CAF NMR Facility during 2017 and 2018, according to the different categories of clients.

Income	2015	2016	2017	2018	2019 projection
SU invoicing	669 227	847 097	656 004	697 665	745 865
External invoicing	478 053	500 894	967 805	641 179	1 015 932
• Commercial				541 818 (190)*	863 542
• Academic				99 361 (1711)*	152 390
Total Income	**R1 147 279**	**R1 347 991**	**R1 623 809**	**R1 338 844**	**R1 761 257**

Expenses					
Salaries	932 580	1 099 918	1 149 123	1 342 756	1 449 464
Running costs	295 759	296 141	359 470	383 393	427 582
Maintenance	40 184	63 570	7 377	12 678	58 297
Travel Costs	1 271				5 140
Small Equipment			33 576		
Total Expenses	**1 269 794**	**1 459 629**	**1 549 546**	**1 738 826**	**1 940 483**

Cost-effectiveness	0,9	0,92	1,05	0,77	0,91

Table 1: Income and expenses of the CAF NMR Facility from 2015 to 2018 and a projection for 2019.
*number of single sample, multi-experimental runs in brackets

practical session. Equipping users with the necessary insight and understanding creates interest and ensures increased equipment utilisation and a growing client base.

Most instrument hardware repairs and general troubleshooting are done in-house, in consultation with either local or remote Agilent NMR support personnel. A reliable specialist solid state NMR service is also provided without the need for an additional appointment for this highly advanced instrument. An existing preventative maintenance schedule is in place for all the spectrometers and supporting infrastructure. Maintenance and usage of logbooks are standard practices. The careful monitoring of these instruments and supporting infrastructure components has contributed to the facility's success.

Industry clients: An Italian tale of coal profiling using CAF Solid-State Nuclear Magnetic Resonance

The NMR Facility has attracted the interest and regular support of a wide variety of industry clients, one of whom is Dr Vincenzo Panebianco. He is a qualified CFD & Combustion Engineer at AC Boilers S.p.A, the largest Italian boiler manufacturer and one of the largest worldwide. In cooperation with a team of engineers and scientists, Dr Panebianco designed a highly efficient low NOx 35MW pulverised coal burner using both advanced mathematical coal devolatilisation and combustion models as a powerful tools to assist in their burner design process. The coal devolatilisation model, in particular, needed five accurate coal lattice parameter values as input. These coal parameter values had to be accurately measured to receive trustworthy predictions about burner performance for steering the engineering process.

In the past, coal lattice parameters had simply been estimated from the available literature, obtaining in return only qualitative predictions rather than quantitative data, which limited the potential of the combustion code. Dr Panebianco needed an alternative to determine the coal lattice parameters accurately, and came across Solid State 13C NMR as a viable analytical tool to determine this. He searched far and wide for a NMR laboratory providing such a service. Eventually, he was pointed in the right direction and scheduled a visit to CAF's NMR Facility in mid-2018.

The SS NMR method the facility adapted and reinstated in-house, from Solum et al., Energy and Fuels, 2001, relies on the recording of two specific semi-quantitative carbon-13 SS NMR spectra. They are defined as a 13C CP MAS and Dipolar Dephased CP MAS NMR experiments with coal-customised parameters. The resulting, seemingly featureless, spectra of the coal are integrated into seven to ten specific regions which in turn are assigned different carbon functionalities in the coal sample (Figure 2,3).

From these specific integral regions a long list of 16 specific coal fractions can be calculated. These range from the fraction aromatic carbons, aliphatics, phenolics and aromatic bridgehead carbons to oxygen-bonded carbons and carbonyls, to name only a few. The values thus obtained for these coal fractions are in turn used to calculate the required Coal Lattice Parameters of the coal sample that are needed as modelling input for the combustion process.

Five of the seven lattice parameters were then fed into the newly developed modelling program to boost the accuracy of the design process, which would otherwise not have been reliable. The mathematical model predicted a confined and highly stable flame shape and oxidiser flow as illustrated in Figure 4, as well as a high overall burner combustion efficiency.

Several months later the design and first full-scale prototype of the coal burner (Figure 5) had been completed and were ready for testing. The burner was mounted and wired at the Gioia del Colle test facility in southern Italy. Accurate in-flame and chimney measurements were recorded in order to assess if the modelled combustion predictions, obtained from the coal NMR analysis, were correct.

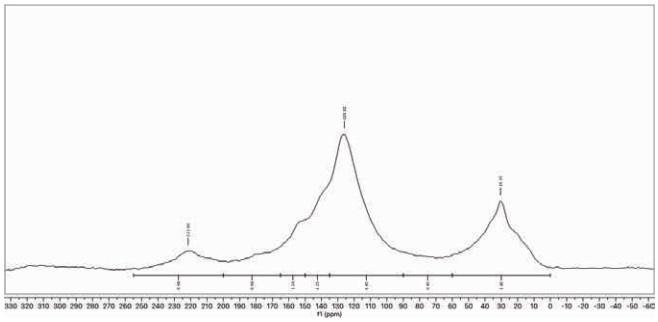


Figure 2: 13C CP spectrum at 12kHz magic angle spinning (MAS) of a typical demineralised coal sample.

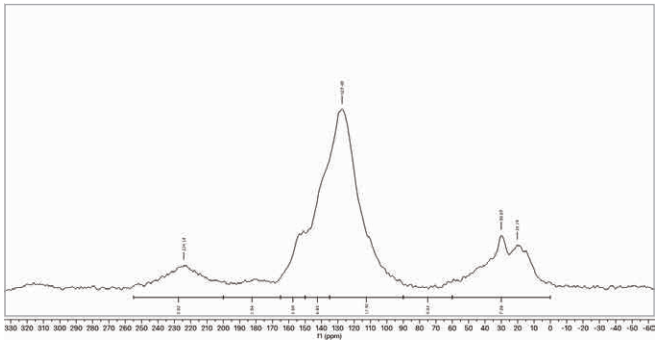


Figure 3: 13C CP with dipolar dephasing spectrum at 12kHz MAS of a typical coal sample (protonated carbons are 'suppressed' during a pre-determined dephasing period).

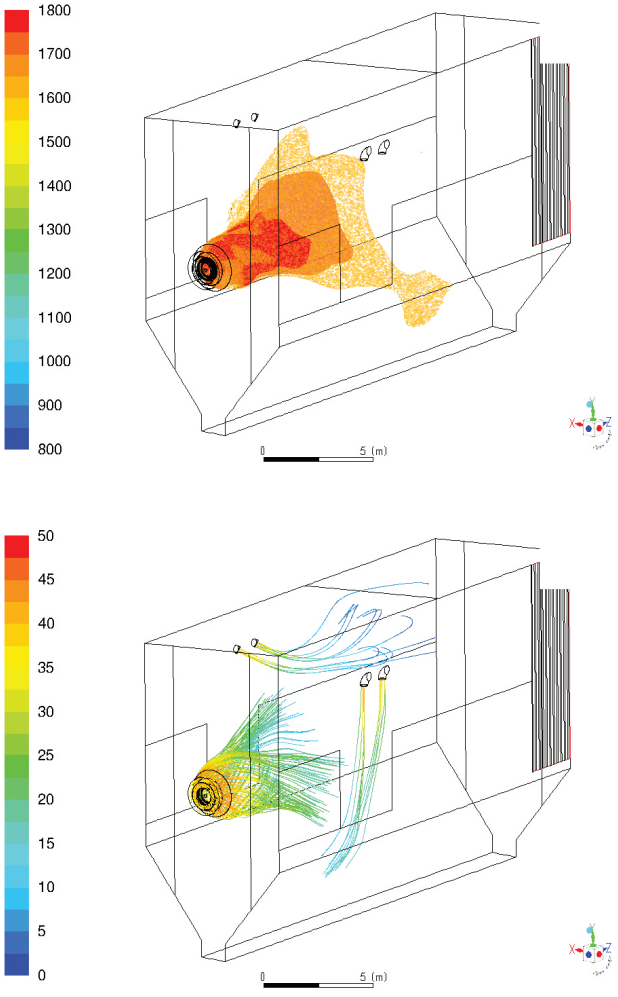


Figure 4: Flame shape contour coloured by temperature [K] (top) and oxidiser flow pathlines coloured by velocity [m/s] (bottom).

Figure 5: Full-scale 35 MW pulverised coal burner at manufacturing facilities during assembling process.

There was great excitement when months of painstaking work by Dr Panebianco came together and paid off. The predicted flame shape and temperature profile from the model were remarkably similar to the observed flame and exceptionally stable (Figure 6). The overall performance of the burner/predictions in relation to NOx, CO, efficiency and unburnt carbon, were also remarkably good.

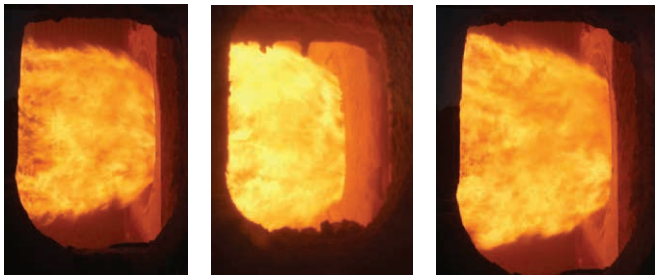


Figure 6: Pictures of the flame front in the near burner field taken at three different times.

The actual 2019 burner results are still confidential (July 2019), but the in-flame measurements and exhaust output data of the same coal in an older 2008 burner, showed an excellent match when using the newly developed mathematic combustion modelling. Using the coal lattice parameters calculated from the SS NMR coal profiling, the new coal combustion model was then successfully validated on both their 2008 and 2019 burners and can now be used to predict and demonstrate to their clients the suitability and expected output from different coals worldwide. Moreover, the combustion model will also be used as a powerful design tool for future multi-fuel Ac-Boilers burners, effectively reducing the time-to-market of new products. Dr Panebianco interacted with various CAF and engineering laboratories during his visit to Stellenbosch with the aim to perform future coal analysis at SU.

Conclusion

Several important components have contributed to the success of the NMR Facility. A diverse client base, effective use of instrument time, cost-effectiveness, innovative administration and industry clients are some of the most important components. A sustainable facility was not built overnight. Doing the right things year after year lead to the favourable position in which the NMR Facility now finds itself.

Financial Reports

By Fransien Kamper

		January 2016-31 December 2016	January 2017-31 December 2017	January 2018-31 December 2018	2019 Projection
MS UNIT	Internal invoicing	1 969 796	2 463 824	2 040 163	1 459 658
	External invoicing	4 754 380	5 379 758	5 148 560	6 818 463
	Total income	6 724 176	7 843 582	7 188 723	8 278 121
	Salaries	2 787 168	2 963 154	3 708 383	4 089 907
	Running costs	1 042 577	969 322	906 574	1 303 626
	Maintenance	632 923	789 232	829 955	515 629
	Travel costs	948	36 784	11 805	481
	Small equipment & KKW	91 539	24 511	70 461	10 952
	Total expenses	4 555 155	4 783 002	5 527 178	5 920 594
FM UNIT	Internal invoicing	848 044	926 172	1 261 988	775 736
	External invoicing	39 136	155 292	74 017	63 212
	Total income	887 180	1 081 464	1 336 005	838 948
	Salaries	1 056 051	1 034 828	889 764	846 166
	Running costs	218 819	259 077	313 664	243 449
	Maintenance	38 610	16 393	79 978	161 480
	Travel costs	9 468	7 025	3 674	17 761
	Small Equipment & KKW	4 686		36 455	107 851
	Total expenses	1 327 634	1 317 323	1 323 535	1 376 707
SEM UNIT	Internal invoicing	656 850	648 946	948 918	892 720
	External invoicing	913 020	1 520 116	2 107 221	849 211
	Total income	1 569 870	2 169 062	3 056 139	1 741 931
	Salaries	1 049 188	1 397 948	2 100 941	1 759 574
	Running costs	143 704	97 459	196 673	139 948
	Maintenance	98 971	436 073	35 975	60 367
	Travel costs	14 476	26 348	64 975	4 858
	Small Equipment & KKW	131 804	91 666	177 800	218 259
	Total expenses	1 438 144	2 049 494	2 576 365	2 183 006

		January 2016-31 December 2016	January 2017-31 December 2017	January 2018-31 December 2018	2019 Projection
ICP & XRF UNIT	Internal invoicing	761 409	860 114	1 045 643	624 936
	External invoicing	1 828 224	2 230 688	2 759 674	3 396 910
	Total income	2 589 633	3 090 802	3 805 317	4 021 846
	Salaries	1 533 321	1 995 338	2 417 316	2 675 160
	Running costs	591 558	727 564	857 977	1 223 638
	Maintenance	232 660	216 324	539 500	1 066 605
	Travel costs	95 634	20 225	77 034	15 094
	Small equipment & KKW	4 642	116 450	29 597	95 301
	Total expenses	2 457 816	3 075 902	3 921 424	5 075 797
DNA UNIT	Internal invoicing	3 198 595	3 805 695	4 690 289	4 772 843
	External invoicing	4 902 329	4 830 122	6 259 800	5 909 985
	Total income	8 100 924	8 635 818	10 950 090	10 682 828
	Salaries	2 301 652	2 440 238	2 986 764	3 034 643
	Running costs	4 382 754	4 445 734	6 669 796	6 285 114
	Maintenance	199 323	317 250	255 726	40 938
	Travel costs	916	2 780	774	
	Small equipment & KKW	186 512	94 901		33 689
	Total expenses	7 071 156	7 300 903	9 913 060	9 394 385
NMR UNIT	Internal invoicing	847 097	656 004	697 665	745 865
	External invoicing	500 894	967 805	641 179	1 015 392
	Total income	1 347 991	1 623 809	1 338 844	1 761 257
	Salaries	1 099 918	1 149 123	1 342 756	1 449 464
	Running costs	296 141	359 470	383 393	427 582
	Maintenance	63 570	7 377	12 678	58 297
	Travel costs				5 140
	Small equipment & KKW		33 576		
	Total expenses	1 459 629	1 549 546	1 738 826	1 940 483
CT UNIT	Internal invoicing	445 672	528 663	663 253	459 100
	External invoicing	1 595 162	1 886 564	2 764 088	1 730 177
	Total income	2 040 834	2 415 226	3 427 341	2 189 277
	Salaries	1 083 401	1 147 982	1 563 400	1 729 619
	Running costs	176 930	359 553	408 092	410 206
	Maintenance	550 312	317 000	313 044	1 047 346
	Travel costs	55 697	75 088	24 491	67 135
	Small equipment & KKW	21 406	64 287	42 057	
	Total expenses	1 887 746	1 963 910	2 351 084	3 254 306

		January 2016-31 December 2016	January 2017-31 December 2017	January 2018-31 December 2018	2019 Projection
NEURO-MECHANICS UNIT	Internal invoicing	463 998	494 473	569 253	559 980
	External invoicing	534 742	702 577	826 252	1 077 157
	Total income	998 740	1 197 050	1 395 504	1 637 137
	Salaries	748 201	1 225 596	1 475 937	2 060 181
	Running costs	139 797	179 398	46 213	114 046
	Maintenance	25 779		66 010	24 864
	Travel costs		34 680	15 589	55 468
	Small equipment & KKW	143 845	25 713	55 196	36 824
	Total expenses	1 057 622	1 465 387	1 658 945	2 291 383
VIBRATIONAL SPECTROSCOPY UNIT	Internal invoicing			57 175	78 304
	External invoicing			18 264	15 617
	Total income			75 439	93 921
	Salaries		33 924	407 321	216 085
	Running costs			7 636	3 787
	Maintenance				
	Travel costs				
	Small equipment & KKW				
	Total expenses		33 924	414 957	219 872
TOTAL UNITS INCOME	Total internal income	9 191 460	10 383 891	11 974 346	10 369 142
	Total external income	15 067 887	17 672 923	20 599 056	20 876 123
	Total income: All units	24 259 347	28 056 814	32 573 402	31 245 265
ADDITIONAL INCOME					
	Interest received	658 894	1 050 629	465 843	1 024 952
	Funds received VR(R)	1 000 000	750 000	750 000	750 000
	Salary contribution VR(R)	3 392 970	3 596 548	3 952 335	3 992 354
	VAT refund on equipment	772 588	128 910		
	Infrastructure NII repayment				2 000 000
	TOTAL ADDITIONAL INCOME	5 824 452	5 526 087	5 168 178	7 767 306
TOTAL INCOME		30 083 799	33 582 901	37 741 580	39 012 571

		January 2016-31 December 2016	January 2017-31 December 2017	January 2018-31 December 2018	2019 Projection
EXPENDITURE	TOTAL EXPENDITURE				
	Salaries				
	Salaries: Admin	1 558 230	1 827 860	1 983 822	2 134 238
	Salaries: Units	11 658 900	13 388 130	16 892 583	17 860 798
	Salaries: Bonus	299 718	366 750	299 326	
	17% / 20% ICRR (indirect cost recovery)	2 561 541	3 004 397	3 501 840	4 175 225
	Running costs (sum of units)	6 992 280	7 397 578	9 790 017	10 151 397
	Maintenance (sum of units)	1 842 148	2 099 649	2 132 866	2 975 525
	Travel costs (sum of units)	177 139	202 930	198 342	165 937
	Small equipment & KKW (sum of units)	584 434	451 104	411 566	502 876
	CAF general running costs	473 143	748 646	674 184	424 577
	CAF-funded post-graduate students				365 991
	Travel costs - courier	72 556	77 797	80 034	63 702
	Development of new labs		415 719		
	Infrastructure	1 262 331	92 912	29 989	
	Infrastructure NII		2 000 000		
	Equipment	931 176	904 483	608 733	874 942
	Equipment repair fund	500 000	500 000	500 000	
	CAF vehicle fund	20 000	45 000	45 000	
	Loan VR(R)	540 000			
	Total normal operational costs	29 473 596	33 522 955	37 148 302	39 695 208
	Surplus per year	610 203	59 946	593 278	-682 637
	CAF overdraft (Originally 5Rmill facility)	3 500 000			
EQUIPMENT EXPENDITURE					
	NRF-NEP total grants	17 300 000	10 237 142		24 720 487
	ALT/US funds	6 217 076	5 127 016		8 000 000
	Departments, faculties, VR(R) contributions	647 806			
	CAF contribution	1 093 910	163 810		871 213
	TOTAL EQUIPMENT EXPENDITURE	25 258 792	15 527 968		33 591 700

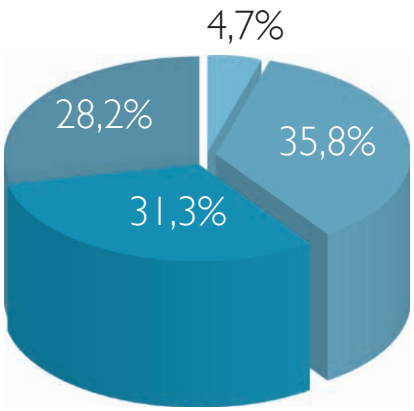
		January 2016-31 December 2016	January 2017-31 December 2017	January 2018-31 December 2018	2019 Projection
NEP EQUIPMENT DETAILS					
	Integrated real-time neurophysiological and biomechanical analysis system	9 520 169			
	Capillary sequencer	4 074 549			
	Waters ultra-performance convergence chromatograph (UPC2) connected to a Waters Xevo TQ-S MS	11 664 074			
	BD FACSMelody cell sorter		7 380 393		
	LabScanner, Prediktera Software and Via-Spec transmission access		8 147 575		
	Mass-directed auto purification & QC system				9 431 805
	Amnis Image StreamX MarkII imaging flow cytometer				12 649 186
	Gemini 300FESEM with advanced system for automated 3D				14 999 739
	TOTAL NEP EQUIPMENT	25 258 792	15 527 968		37 080 730

FUNDS					
	Emergency equipment repair fund	1 036 543	1 353 701	1 582 635	500 000
	Vehicle replacement	59 686	108 464	160 930	165 000
	Reserve, food security project	1 109 835	1 188 095	1 201 041	1 202 000
	Maintenance fund equipment: BD FACS Jazz sorter (2013)	1 168 049	1 250 413	1 185 280	1 194 989

NODE FOR INFECTION IMAGING UNIT Total project costs not only funds managed by CAF	Start-up funding				63 985 810
	Interest received				4 197 671
	Total income				68 183 481
	Salaries & running costs				1 792 713
	Building & equipment				59 147 697
	CAF contribution repay				2 000 000
	Operating costs				5 243 000
	Total expenses				68 183 410

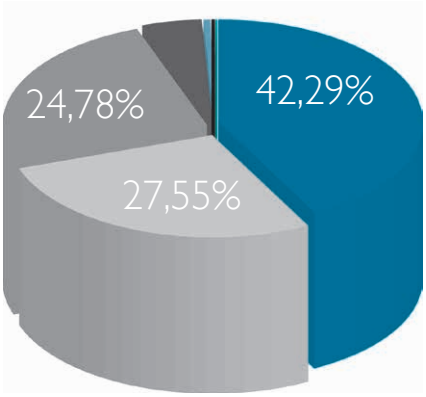
Graphs detailing aspects of CAF income during 2018

2018 income derived from the four main categories of clients:



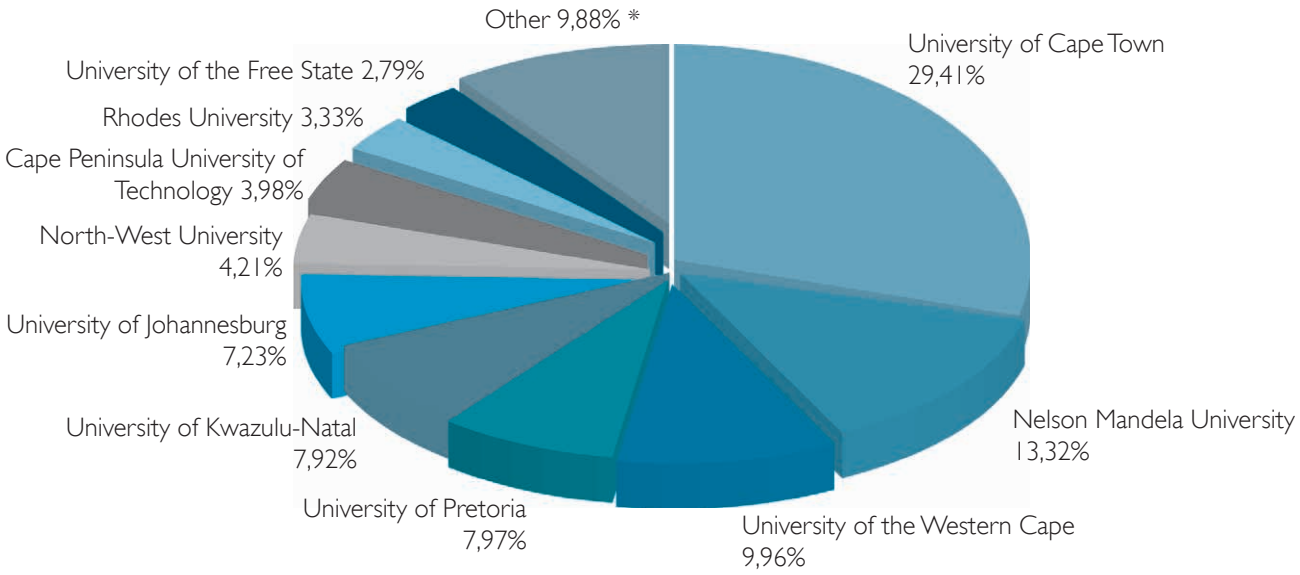
- SU clients 35,8%
- Industry clients 31,3%
- Clients from other SA universities 28,20%
- International client 4,70%

Analysis of CAF income from internal clients by faculty:



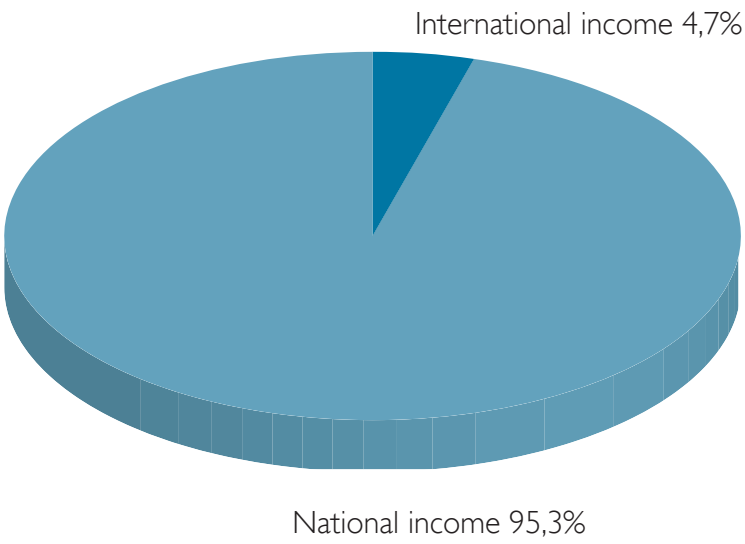
- Faculty of Science 42,29%
- Faculty of AgriSciences 27,55%
- Faculty of Medicine & Health Sciences 24,78%
- Faculty of Engineering 4,81%
- Faculty of Education 0,53%
- Military Science 0,03%
- School of Public Leadership 0,01%

Analysis of CAF income from South African external academic clients by university:



* Other: Rhodes University, University of the Witwatersrand, Central University of Technology, University of Venda, University of Fort Hare, University of Limpopo, UNISA, Tshwane University of Technology, Vaal University of Technology, Walter Sisulu University, Durban University of Technology, University of Zululand

Analysis of the proportion of CAF income from external clients that is derived from international clients:



CAF structure 2019

MANAGEMENT
Director: Prof Gary Stevens • Manager: Mrs Fransien Kamper

Mass Spectrometry Unit
Dr Marietjie Stander

GCMS | LCMS | Proteomics | Biomedical

DNA Sequencing Unit
Mr Carel van Heerden

DNA sequencing/ fragment analysis | NGS

Electron Microscopy Unit
Prof Lydia Joubert

Nuclear Magnetic Resonance Unit
Dr Jaco Brand

Fluorescence Microscopy Unit
Mrs Lize Engelbrecht

CT Scanner Unit
Prof Anton du Plessis

NuMeRI Node for Infection Imaging (NII)
Dr Alex Doruyter

NII, a part of the Nuclear Medicines Research Infrastructure that is managed by CAF, will function on a different financial basis than the CAF units. CAF supports NII financially when needed and NII repays this money to CAF as earnings accrue. Once NII is profitable, profits flow to NuMeRI.

Neuromechanics Unit
Dr John Cockcroft

ICP-MS & XRF Unit
Mrs Riana Rossouw

ICP-MS & XRF | Geochronology

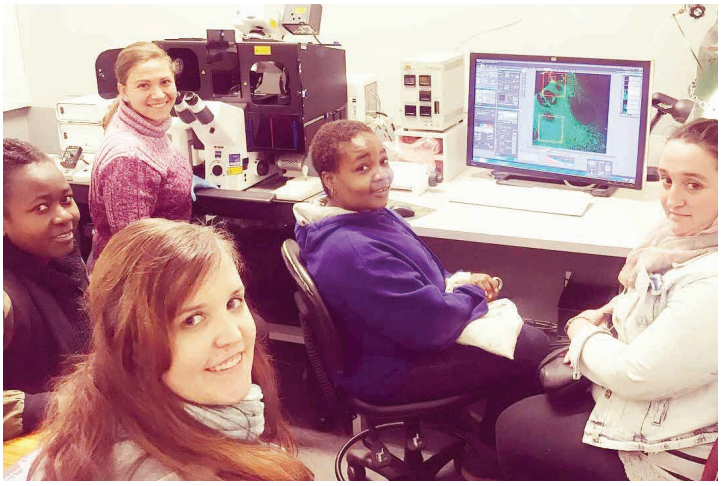
Vibrational Spectroscopy Unit
Dr Janine Colling

PLEASE NOTE: Names of the unit managers are indicated in dark blue blocks and divisions within units are indicated in light blue blocks.

Addendum 1

Training Initiative: 24–28 June 2019
Report and overview

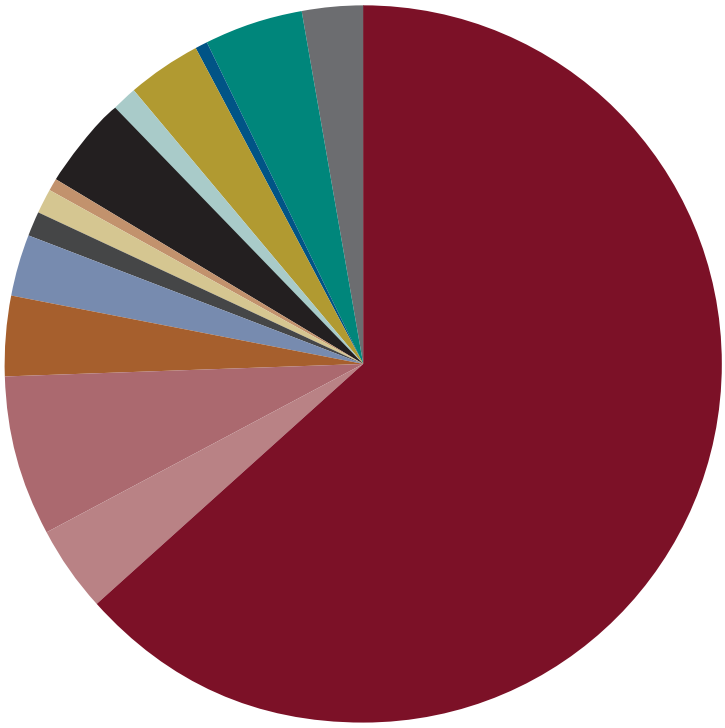


CAF is in a unique position to provide high-quality, hands-on training in the use and functioning of a range of high-end analytical equipment not readily available at all universities in South Africa. Consequently, CAF runs an annual training event to address the considerable need for training in analytical techniques that exists at South African universities. At the 2019 annual Training Initiative 17 different workshops were presented. See the table below indicating the dates on which each workshop took place as well as the number of people who registered and attended.

WORKSHOPS	JUNE 2019					Registered	Attended
	24	25	26	27	28		
Introduction to U-(Th)-Pb Geochronology by LA ICP-MS by Dr Laura Bracciali (1 day)				27		10	10
Practical XRF Spectrometry (1 day) by Mrs Mareli Moolman			26			16	13
Solution ICP-MS in Environmental analysis of major and trace elements (1 day) by Mrs Riana Rossouw		25				10	9
Introduction to Hyperspectral imaging and chemometrics (2 days) by Dr Janine Colling	24	25				6	6
Nucleic Acid Preparation, QC and Library building for Next Generation Sequencing (4 days) by Ms A Vorster and Mr CJ van Heerden	24	25	26	27		12	12
Cell Sorting on the BD FACS Melody (1 day) by Mrs Lize Engelbrecht	24					6	6
Super-resolution Microscopy: SR SIM and PALM/STORM (1 day) by Mrs Lize Engelbrecht		25				6	6
Correlative Light and Electron Microscopy (1 day) by Mrs Lize Engelbrecht and Prof Lydia-Marie Joubert			26			6	4
Biological Electron Microscopy: Basic Principles and Advanced Applications (1 day) by Prof Lydia-Marie Joubert		25				8	8
Introduction to Analytical Electron Microscopy (1 day) by Prof Lydia-Marie Joubert and Ms Madelaine Frazenburg				27		8	8
Solution State Nuclear Magnetic Resonance Spectroscopy (1 day) by Dr Jaco Brand	24					6	5
Introduction to X-ray Micro- and Nano-CT (1 day) by Ms Muofhe Tshibalanganda		25				10	6
Noraxon mobile neuromechanical analysis (kinematics, kinetics and EMG) (2 days) by Dr John Cockcroft, Ms Tamsin Purkis, Ms Cara Mills, Dr Lara Grobler				27	28	6	5
Vicon neuromechanical analysis (kinematics, kinetics and EMG) (2 days)by Dr John Cockcroft, Ms Tamsin Purkis, Ms Cara Mills, Dr Lara Grobler	24	25				5	4
Mass Spectrometry of Small Molecules: LC-MS (1 day, 2 different groups 1 day each) by Mr Erick van Schalkwyk and Mr Malcolm Taylor	24	25				43	37
Mass Spectrometry of Small Molecules: GC-MS (3 days) by Mr Lucky Mokwena and Mr William Arries			26	27	28	40	30
Mass Spectrometry Based Proteomics (3 days) by Dr Maré Vlok			26	27	28	10	10
						Total participants 2019:	179

Training Initiative attendance - SU (internal) participants and external participants



Stellenbosch University 113 — **Internal: 113**

University of Fort Hare 7
University of the Western Cape 13
Industry (Fine Chemicals, DNA Biotec, NHLS) 6
Cape Peninsula University of Technology 5
North-West University 2
University of Botswana 2
University of Venda 1
Vaal University of Technology 7
University of the Witwatersrand 2
Central University of Technology 6
Tshwane University of Technology 1
University of Cape Town 8
University of Namibia 5

— **External: 66**

Advertising

Information about the Training Initiative and the invitation to apply were distributed to the following groups of people:

- All internal and external clients on the CAF database.
- The Division of Research Development (Aasima Gaffoor) distribution list.
- The African Doctoral Academy (Corinna du Toit) newsletter and electronic advertisements.
- The Tygerberg Campus (Hermien Nel) big screens and newsletter.

The CAF website was also updated with all information about the Training Initiative.

Applications

Participants applied by completing an online form created in Machform. They had to select a first-option and second-option workshop. The form was set up in a way that only second-option workshops that did not clash (in terms of the date) with the first-option choice were visible after selecting the first-choice workshop. This helped with the administration and there was no need to check for clashes manually. More than 200 applications were received (some applying for more than one workshop).

Finances

Expenses:
Stias Opening Dinner (25 June): R43 425 (booked for 115, about 110 attended)
Programme and menu prints: R243-00

Brochures, notepads and certificates were printed, but not only for use at the Training Initiative.

Income:
Industry attendees x 6 @ R5 000 each = R30 000
The Division of Research Development contributed R6000 in support of Early Career Development participants.

Displays at the Welcome Dinner

Sponsors had the opportunity to have displays at the Welcome Dinner at Stias. Separations, ThermoFisher, Zeiss, Perkin Elmer, LecoAfrica and Labotec made use of this opportunity.

Other

Presenters received a box with attendance lists, brochures, notepads, pens and certificates for each workshop.

Comments

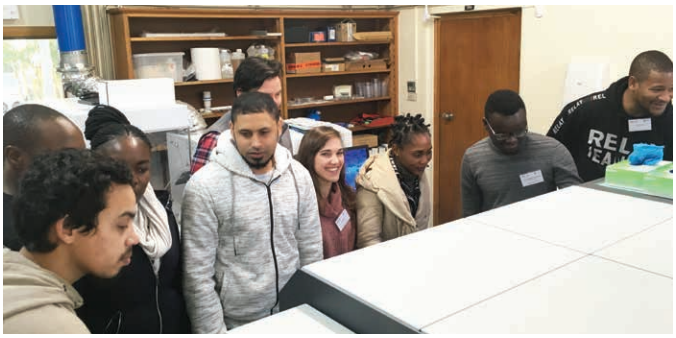
Last year several registered participants did not show up for their workshops. In an endeavour to prevent this from happening again, we included an option in the registration form for people who wanted to attend but were unsure whether they would be able to. By doing this we were able to follow up with those particular participants and give someone else the opportunity to attend. Participants also realised that by registering for a workshop they committed themselves to show up.

Conclusion

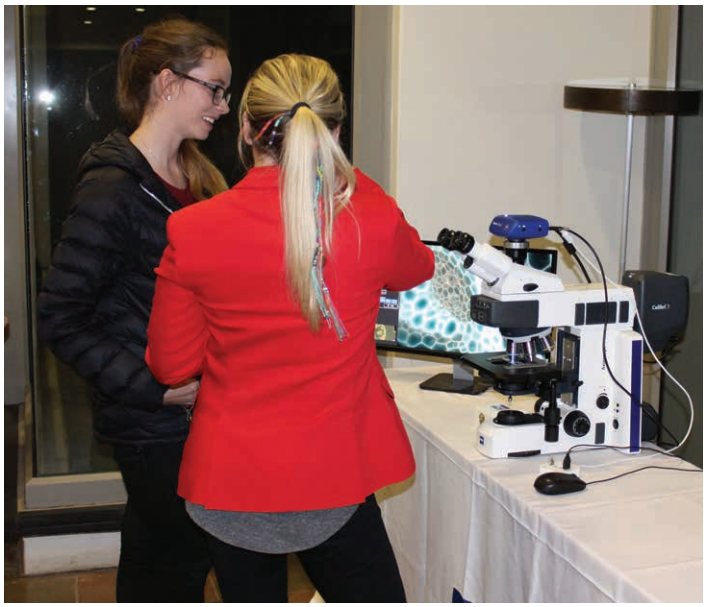
The Training Initiative notice was sent to a larger number of possible participants this year and consequently significantly more people applied for workshops. Only 108 people attended workshops in 2018, while 179 people attended in 2019. Some of the workshops did not have enough space to accommodate everyone who applied.


LABOTEC
Laboratory Solutions Across Africa
www.labotec.co.za


ThermoFisher
SCIENTIFIC




CAF
advancing research
www.sun.ac.za/caf



First notice sent by email

get trained

high quality, hands-on training on the use and functioning of a range of high-end analytical equipment

by the Central Analytical Facilities (CAF) at Stellenbosch University

CAF Central Analytical Facilities STELLENBOSCH UNIVERSITY

UNIVERSITEIT iYUNIVESITHI STELLENBOSCH UNIVERSITY 100 1918·2018

save the date

24 – 28 June 2019

online applications
open: 11 April 2019
close: 6 May 2019
www.sun.ac.za/caf

workshops:

Introduction to Hyperspectral imaging and chemometrics
by Dr Janine Colling (2 days)

Vicon neuromechanical analysis (kinematics, kinetics and EMG)
by Dr John Cockcroft, Ms Tamsin Purkis, Ms Cara Mills and Dr Lara Grobler (2 days)

Noraxon mobile neuromechanical analysis (kinematics, kinetics and EMG)
by Dr John Cockcroft, Ms Tamsin Purkis, Ms Cara Mills and Dr Lara Grobler (2 days)

Solution State Nuclear Magnetic Resonance Spectroscopy
by Dr Jaco Brand (1 day)

Introduction to X-ray Micro- and Nano-CT
by Ms Muofhe Tshibalanganda (1 day)

Solution ICP-MS in Environmental analysis of major and trace elements
by Mrs Riana Rossouw (1 day)

Practical XRF Spectrometry
by Mrs Mareli Grobbelaar-Moolman (1 day)

Introduction to U/Pb Geochronology and data processing
by Dr Laura Bracciali (1 day)

Nucleic Acid Preparation, QC and Library building for Next Generation Sequencing
by Ms A Vorster and Mr CJ van Heerden (4 days)

Cell Sorting on the BD FACS Melody
by Mrs Lize Engelbrechy (1 day)

Super-resolution Microscopy: SR SIM and PALM/STORM
by Mrs Lize Engelbrecht (1 day)

Correlative Light and Electron Microscopy
by Mrs Lize Engelbrecht and Prof Lydia-Marie Joubert (1 day)

Biological Electron Microscopy: Basic Principles and Advanced Applications
by Prof Lydia-Marie Joubert (1 day)

Introduction to Analytical Electron Microscopy
by Prof Lydia-Marie Joubert, Ms Madelaine Frazenburg and Dr Elrika Harmzen-Pretorius (1 day)

Mass Spectrometry of Small Molecules: LC-MS
by Mr Erick van Schalkwyk and Mr Malcolm Taylor (1 day)

Mass Spectrometry of Small Molecules: GC-MS
by Mr Lucky Mokwena and Mr William Arries (3 days)

Mass Spectrometry Based Proteomics
by Dr Maré Vlok (3 days)

PLEASE NOTE:

- **Exposure** to equipment to reinforce theoretical principles.
- **Develop** the necessary practical skills.
- **Data interpretation** will also be covered in most workshops.
- **Aimed at** postgraduate students, researchers, university and industry technical staff.
- **Places** are limited due to space constraints in laboratories for hands-on exposure to equipment.
- **Preference** to applicants who can motivate that their participation will directly benefit their own research or the research of others.
- **A final outline and scheduling** of the workshops will follow in April 2019 on our website: *www.sun.ac.za/caf*
- **Online Applications (www.sun.ac.za/caf) open 11 April and close 6 May.**
- Certificates of participation will be issued at the end of the workshop.
- All researchers, postgraduate students and university and industry technical staff may apply.
- Participants may apply for a maximum of 2 workshops, provided these do not clash in terms of scheduling. In the event of a conflict the first workshop will be selected.
- **The training is free to staff and students at South African universities.**
- **Participants from industry will be charged R5000 per workshop.**
- Participants must make their own travel and accommodation arrangements.
- Travel, accommodation and meal expenses are for the participant's or their institution's own cost.
- The successful candidates will be notified by e-mail no later than 22 May 2019.

www.sun.ac.za/caf

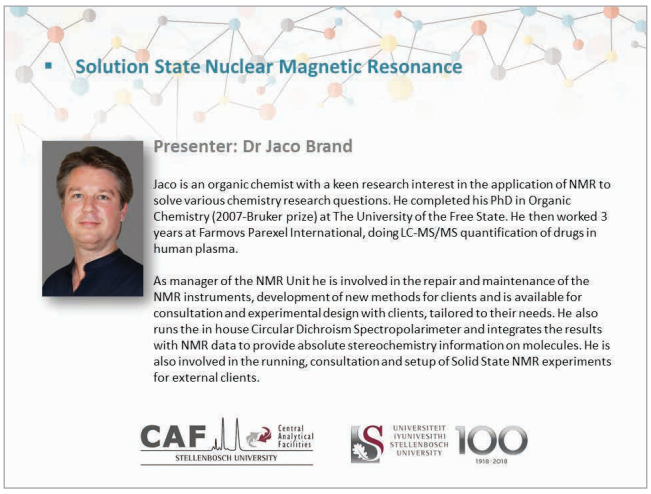
Second notice

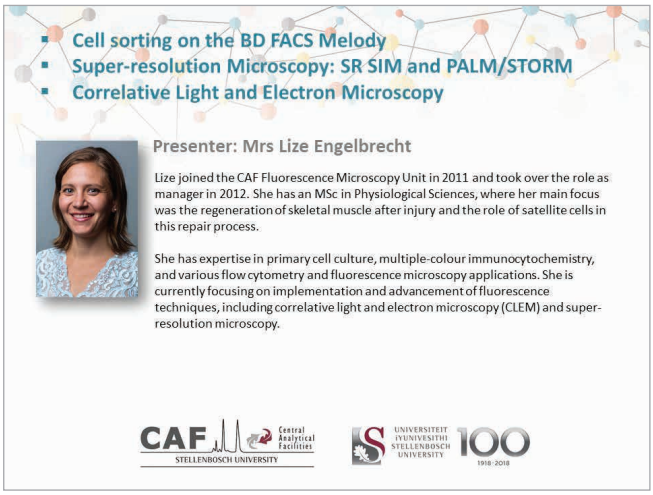
Invitation to Welcome Dinner

Reminder Welcome Dinner

Programme and menu Welcome Dinner

Slides from PowerPoint Presentation at Welcome Dinner






LABOTEC
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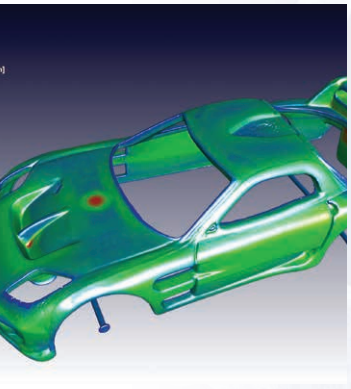
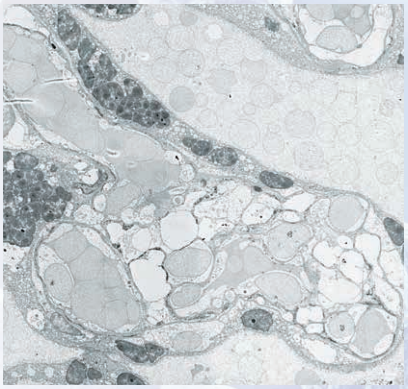
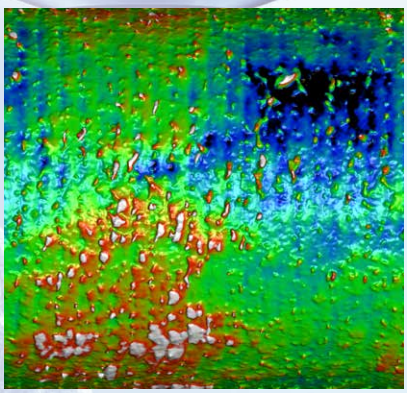

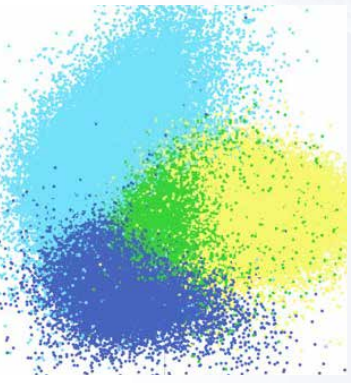
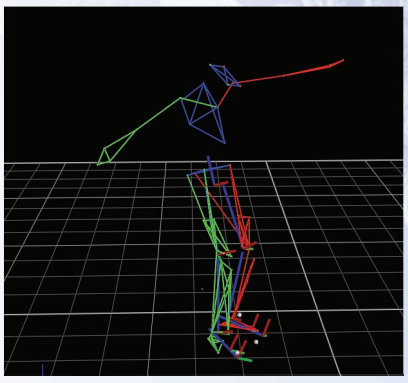

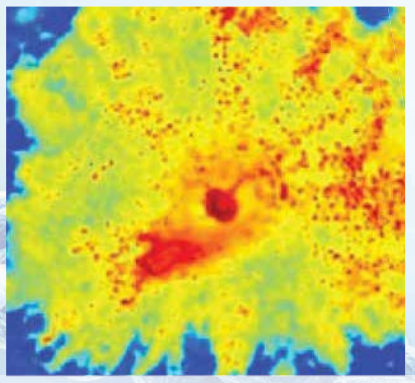

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