

## Annual Report for EPSRC Mid-Range Facilities

Facility: EPSRC National Crystallography Service

Address: NCS, Chemistry, University of Southampton, Highfield Campus, University Road, Southampton, SO17 1BJ

Director: Professor Simon Coles

Facility Manager: NCS Operations Manager, Dr Graham Tizzard; NCS Service Support Manager, Sarah Milsted: EPSRC Manager, Sally Birse.

### Description of the Facility

The NCS facility is amongst the most powerful and highest throughput of its type in the world. Its core business is to handle and examine samples that a typical academic crystallography unit cannot. The service focusses on the technique of single crystal diffraction applied to samples submitted by UK Chemistry, and related, disciplines. This technique provides the most detailed characterisation possible for solid-state chemicals and the NCS is dedicated to investigating the smallest and weakest scattering crystals that challenge the community. In addition to structure determination the NCS also provides advanced crystallographic studies using charge density, variable temperature, high pressure and gas cell techniques. A commercial service for the industrial sector is also available.

Professionalism is a trademark of the NCS – it prides itself in exemplary and rigorous processes for sample handling and tracking, data management and publishing, a bespoke user interface and an ability to deliver to a demanding set of KPIs. Sample turnaround time is exemplary, meaning that this technique is often used to progress research, as well as producing the characterisation of its final outputs. Users can select either raw/derived data being provided for their own analysis, or a full analysis service, where a sample is taken through to publication. The ability to handle the most demanding samples in the Southampton laboratory is a key feature, and provides an effective filter for a follow-on synchrotron service. The NCS has regular access to the world-leading I19 beamline at Diamond Light Source.

The track record of the NCS team is exemplary, with a proven ability to deliver a high profile and high throughput service. The facility has an exceptional publication record and is amongst the world's most prolific contributors to the Cambridge Structural Database. The NCS is well established in the research community and leads in many aspects, both nationally and globally.

### Contract Period and Costs

Contract Term: 3+2 years

Start Date: 01/11/2016

End Date: 31/10/2019 (3 years) / 31/10/2021 (5 years)

Total cost: £3,900,460.96 ex VAT

Total capital cost: £166,024.01 ex VAT

Spend on track? Yes

## Key Performance Indicators (KPIs) and Service Level (SLs)

Type: SL= Service Level, RMI = Reporting and Management Information

Type	Description	Time for Performance	SLA Level			1st Sep 2016 - 31st Aug 2017	Directors Comments
			Green	Amber	Red		
RMI	Total number of all Users	Period associated with specific report	N/A	N/A	N/A	62 (Routine service active users) / 42 (Training schemes)	
RMI	Spectrum of user types	Period associated with specific report	N/A	N/A	N/A	59 (Routine service active users) / 42 (Training schemes) / 3 (Commercial clients) / 2 (Advanced techniques)	
RMI	Number of University / Research Groups Involved	Period associated with specific report	N/A	N/A	N/A	30 (University) / 77 (Research group)	
RMI	Percentage of Access Requests Accepted	Period associated with specific report	N/A	N/A	N/A	100% (Routine service) / 100% (Advanced Technique)	
RMI	Percentage of equipment time dedicated to different access modes	Period associated with specific report	N/A	N/A	N/A	70% (Routine service, academic) / 5% (Commercial) / 20% (Host institution) / 5% (Advanced techniques)	
RMI	The number of data sets processed		N/A	N/A	N/A	869	
SL	Percentage of User enquiries responded to within Stated Window	2 working days	95% and above	>90% but <95%	90% or less	100%	
SL	Percentage of Access Requests Responded to within Stated Window	2 working days	95% and above	>90% but <95%	90% or less	100%	
SL	Percentage of Training Requests Responded to within Stated Window	2 working days	95% and above	>90% but <95%	90% or less	100%	

SL	Percentage of Training Requests Delivered within 3 months	3 months	95% and above	>90% but <95%	90% or less	100%	
SL	Number of Customer Complaints (expressed as a percentage of the Total Number of User Approvals made within the period)	Period associated with specific report	Less than 5%	5-10%	Over 10%	0%	
SL	Percentage of customer complaints resolved within Stated Window using the Dispute Resolution Plan.	Period associated with specific report	95% and above	>90% but <95%	90% or less	n/a	
SL	Percentage Uptime/Downtime per instrument of Total Available Time within Period	Period associated with specific report	95% and above	>90% but <95%	90% or less	Mo FRE+ VHF 89.6%	The FRE+ x-ray generator suffered a water seal failure which required substantial maintenance/repair work (carried out immediately and under warranty) and subsequent realignment. This accounts for the majority of the downtime on the FRE+ based instruments.
SL	Percentage Uptime/Downtime per instrument of Total Available Time within Period	Period associated with specific report	95% and above	>90% but <95%	90% or less	Mo FRE+ HF 91.6%	
SL	Percentage Uptime/Downtime per instrument of Total Available Time within Period	Period associated with specific report	95% and above	>90% but <95%	90% or less	Cu 007 HF 94.4%	Both the FRE+ VHF and Cu007 instruments underwent significant detector upgrades during this period, which resulted in planned, announced and managed downtime. A combination of this upgrade and the FRE+ repairs are the cause of the RED KPI - and both of these situations were overcome as expected.
SL	Percentage of Access Costs recovered	Period associated with specific report	10	6	2	n/a this year	
SL	Number of Publications	1 year	30	20	10	51	

SL	Number of publicity activities per year	1 year	10	8	6	10	
SL	The time from arrival of a sample to logging in and informing a User of receipt	within 2 working days	95% and above	>90% but <95%	90% or less	100%	
SL	The time a sample is in the queue	From logging in a sample to examination: High Priority sample = 10 working days	95% and above	>90% but <95%	90% or less	95.10%	
SL	The time a sample is in the queue	From logging in a sample to examination: Medium Priority samples = 20 working days	95% and above	>90% but <95%	90% or less	95.20%	
SL	The time a sample is in the queue	From logging in a sample to examination Low Priority samples = 30 working days	95% and above	>90% but <95%	90% or less	95.10%	
SL	Time from examination to end result	Data collection = 5 working days	95% and above	>90% but <95%	90% or less	95.30%	
SL	Time from examination to end result	Full Structure Analysis= 20 working days	95% and above	>90% but <95%	90% or less	92%	The Amber level is due to staffing shortage. The NCS was operating with one less PDRA from Nov 2016 - Jan 2017, due to the resignation of Dr Mateusz Pitak during the previous tender extension period. Dr Wim Klooster was appointed from 09/01/2017 and was undertaking training and family relocation during the second half of this reporting period.

## Users:

### User statistics.

NCS users in the reporting period fall into four categories:

- a) Research Group Principal Investigators. 54 NCS PI's, of which 8 were new users. A user is defined as a group leader who holds an allocation used by that entire research group.
- b) 8 UK service crystallographers. This usage mode supports large (additional) numbers of researchers as they are departmental crystallographers accessing the NCS to analyse difficult samples from across *their* entire user base.
- c) Collaborators using Advanced Techniques. In the latter stage of the reporting period the first of four Advanced Techniques pilot study areas was launched - Variable Temperature. Charge Density, High Pressure and Gas Environment will be sequentially launched over the coming allocation periods. 2 users performed pilot studies in this period.
- d) Industrial Users. The NCS launched its commercial service towards the end of the reporting period and has served 3 industrial users.
- e) International Collaborations. These are detailed in the International interactions section of this report.

We do not record the number of students for each PI accessing the NCS, however an accepted estimation is that on average a user would have 2-3 students (some groups are into double figures).

The NCS users originate from 36 different institutions. 84% of our users are based in chemistry departments, while the remaining 16% originate from materials science, defence materials, pharmacy and biochemistry departments. The geographic spread of users is even and touches all regions of the UK. User groups cover 13 EPSRC research areas detailed in the strategic fit section of this report.

Some time on the facility equipment is allocated to the host institution (departmental crystallographer, self-service users and Coles group research). The facility is regularly used in training, demonstration and outreach events. Rigaku Oxford Diffraction have used the facility to demonstrate to staff and customers.

### User satisfaction survey

Over 60% of active users (41 respondents) replied to a user satisfaction survey as follows:

- The NCS is easy to use, e.g. ease of application, clear sample forms and guidance [4.78/5]
- The NCS is responsive to user requests, e.g. rapid turnaround, additional data collections [4.96/5]
- The NCS is helpful with regard to publication, e.g. all data necessary provided, assistance with crystallography sections etc. as per type of service requested [4.86/5]
- I would recommend the NCS to a colleague [4.92/5]

Some representative comments illustrating the value of our services to our users include:

- "NCS has been a great support to us in our research progress and we are extremely grateful to be able to access this service. I would always be happy to offer my support to the NCS; it is a real asset to the UK research community."
- "Recently I have needed assistance with the publication of results from previous allocations and the staff have been excellent in providing the support I needed."

The previous survey identified two areas for improvement (consistency of CIFs and online monitoring) and work on addressing these is detailed in the improvements section.

The NCS is in itself an illustration of scientific excellence - the facility is an acknowledged world leader in the field service crystallography and unique in the scale at which it operates.

### Publishing highlights

The record for journal publications in this period is very similar to that of last year. This illustrates sustained excellence as evidenced by our user survey from 2016, which can be summarised thus: The majority of NCS work cannot be done in the home laboratory – 62% of our users have local facilities and yet they still have a strong need for more powerful facilities. Furthermore 50% of NCS structures are published in journals and 74% in a thesis, indicating the high value of NCS data.

A 2012 perspective article on the future direction of crystallography (Coles & Gale, *Chem Sci*, **2012**, 3, 683-689) outlined the NCS operation. As of May/June 2017 this highly cited paper had received enough citations to place it in the top 1% based on Web of Science's highly cited threshold for the publication year and field. In this reporting period 27 co-authored papers were published and this is supplemented by at least the same number of papers also arising from our data collection only service. The top five papers of the period during this period are summarised as:

A switchable self-assembling and disassembling chiral system based on a porphyrin-substituted phenylalanine-phenylalanine motif, NATURE COMMUNICATIONS, DOI: [10.1038/ncomms12657](https://doi.org/10.1038/ncomms12657)

From Ligand to Phosphor: Rapid, Machine-Assisted Synthesis of Substituted Iridium(III) Pyrazolate Complexes with Tuneable Luminescence, CHEMISTRY-A EUROPEAN JOURNAL, DOI: [10.1002/chem.201701551](https://doi.org/10.1002/chem.201701551)

Cyclometalation via Carbon-Fluorine Bond Activation Induced by Silver Particles, ORGANOMETALLICS, DOI: [10.1021/acs.organomet.6b00872](https://doi.org/10.1021/acs.organomet.6b00872)

When Weaker Can Be Tougher: The Role of Oxidation State (I) in P-vs N-Ligand-Derived Ni-Catalyzed Trifluoromethylthiolation of Aryl Halides, ACS CATALYSIS, DOI: [10.1021/acscatal.6b03344](https://doi.org/10.1021/acscatal.6b03344)

A Copper-Benzotriazole-Based Coordination Polymer Catalyzes the Efficient One-Pot Synthesis of (N<sup>1</sup>-Substituted)-hydrazo-4-aryl-1,4-dihydropyridines from Azines, ADVANCED SYNTHESIS & CATALYSIS, DOI: [10.1002/adsc.201601072](https://doi.org/10.1002/adsc.201601072)

### New methodologies developed

The main methodology development has been the installation of the new Hybrid Pixel detectors on two of the instruments. Tests and analyses highlighted in the 2016 annual report indicated to us that this technology would be the next step change for service crystallography. During this period we have been implementing and embedding this technology and our predictions are turning out to be true. The productivity, throughput and capability of the facility is dramatically increased and equally importantly, the data quality is increased too. These upgrades have exceeded expectations and have resulted in close working with the instrument manufacturer to promote this outcome. The first test data collected proved to be a particularly challenging problem that this technology resolved more readily, accordingly we produced an application note with Rigaku, the summary of which was then incorporated into their new product brochure (acknowledging the NCS).

We continue to perform our role as 'horizon scanners' for potential new advances in the field and to this end we hosted a visit from Excillum. This company makes X-ray generators based on an entirely new technology (Liquid Metal Jet) and accurate comparison evaluations were made. The new results indicate that this new technology is indeed worth monitoring and we will be continuing to build links with them.

The renewal tender introduced 'Advanced Techniques' at the NCS. We have spent much of the period devising a timeline to bring them on stream and embarking on this. We have performed our first experiments and the initial results are very promising. Collaborations with Prof Weller (Oxford) relating to monitoring in-situ hydrogenation and

with Drs Blair and McAteer (Cranfield) on the solid-state transformations of nitroglycerine are developing quickly with publication of results and bids for independent funding imminent in the next reporting period.

The NCS work that highlighted the occurrence of radiation induced crystal decay at the Diamond synchrotron and formed a case study in 2015 ([http://www.ncs.ac.uk/files/a8263bc2/NCS case study 1.pdf](http://www.ncs.ac.uk/files/a8263bc2/NCS%20case%20study%201.pdf)) has been built on. Working with the Garman group (Biophysics, Oxford) we have been modifying the approach pioneered by them that has been universally adopted by the macromolecular crystallography community. This work is at an advanced stage and a manuscript is in preparation and it will also form the basis of a global project to investigate this effect at other synchrotrons, two in the US, Germany, Japan & Australia (see also International section of this report).

### **Case studies**

Two case studies have been worked on in this period. The first, from Dr Peter Holliman at Bangor University ([http://www.ncs.ac.uk/files/is2aBPg/NCS Bangor.docx](http://www.ncs.ac.uk/files/is2aBPg/NCS%20Bangor.docx)), is based on designing molecules for light harvesting and charge transport. Solar cells are multi-layer devices and speeding up manufacturing means that each layer of the device needs to rapidly self-assemble on the previous layers to create a perfect molecular jigsaw - NCS data identifies the molecular structures of each part of the solar cell jigsaw and sheds insight into how to design molecules that optimise the way they fit together. Dr Holliman states "Without the NCS it would be impossible for us to continue with our work. We wouldn't be able to get the data we require to proceed and we wouldn't be able to get our work published. If we can't publish anything, our project would grind to a halt".

The second case study is rather different in that it is about the NCS itself. The Science and Engineering South Consortium (SES), which brings together the universities of Oxford, Southampton, King's College London, Queen Mary University of London, University College London and Imperial College London, commissioned the case study. As a hub, the purpose of the consortium is to collaborate and share knowledge, access to facilities and training – a remit that fits well with that of the NCS, which is why we were chosen as an exemplar. The case study is published at <http://www.ses.ac.uk/2017/07/18/crystal-clear-materials/>.

### **Publications for a broader audience**

A central theme of the International Union of Pure and Applied Chemistry (IUPAC) World Chemistry Congress was chemical information. Simon Coles authored two papers that referenced the pivotal role of crystallography acting as an exemplar, where NCS was discussed as an example of best practice. To mark this theme, a special issue of IUPAC's Chemistry International magazine was released and Simon Coles authored two of the fourteen Feature Articles (on Data Sharing in Crystallography & Leveraging the Web to Disseminate Crystallographic Data). There were two further (vide supra) significant contributions to Rigaku brochures one on customer productivity for a general brochure and another on our application of the benchtop instrument to teaching and training.

Training continues to be a key aspect of development for the NCS and Simon Coles made a presentation on our hands-on, problem-led teaching innovations at the American Crystallographic Association meeting (New Orleans, May). Furthermore, introductory YouTube videos on performing Single Crystal and Powder diffraction <https://youtu.be/suVNYD1nCm4> and <https://youtu.be/ZYzKd2qMn1o> were produced and have generated 5800, 4400 views respectively.

### **Work in related areas**

Data Management and Sharing continues to be a key element of the NCS, in which it is an established leader. Simon Coles contributed to the International Union of Crystallography working group in this area, presenting at its final workshop (New Orleans, May). This working group has been disbanded and a new IUCr Commission, CommDat, has been established – Simon is one of the founding 12 members of the committee and attended the inaugural meeting (Hyderabad, August). Simon will be leading a piece of work on raw data publication for small molecule crystallography, which will likely lead to recommendations for the whole global community. EPSRC Impact Acceleration funds have been secured to develop the NCS electronic facility management system, Portal. The project aims to produce and package a generic facility management system for exploitation both by HEIs and also industry.

### Training courses and workshops.

The renewal of NCS funding has a significant training element incorporated and accordingly a training delivery plan has been established. Three major events were conducted during the reporting period:

- Approaches to Modelling Disorder: Hosted by NCS, this workshop ran twice (Apr and May) due to oversubscription. A total of 18 attendees experienced a day of hands-on style workshop, where group working on their own data was particularly valued.
- An Olex2 workshop for intermediate crystallographers in May had 8 attendees
- An invited 1-day workshop for the 'ResMoSys' Innovative Training Network in Cambridge taught 16 chemists how to better exploit crystallographic results to further their research.
- The Director assisted in the Rigaku "Live Labs" at the IUCr Congress, where many students from developing nations were introduced to hands-on crystallography for the first time.

Formal feedback gathered from the attendees of all these courses has informed the topic of the next workshop (Handling Twinning – aimed at intermediate/expert crystallographers).

### Activities to promote the facility beyond its core user base.

The Director has promoted the NCS to a number of different audiences outside of the existing/core user base. In September a Plenary talk at the recent appointees in UK Inorganic Chemistry (MICRA, Bath) addressed an audience of around 100, which rose awareness across the UK and generated leads for advanced techniques experiments. The NCS sponsored the RSC Dalton Southern area meeting in June, where the Director was the judge of posters and presentations, speaking with around 80 early career chemists.

### Public engagement.

In April Sarah Milsted was awarded a BCA Outreach Bursary to develop resources for Primary Schools Outreach and the NCS took on a BCA-funded project to develop an open online repository to host outreach resources.

The NCS was involved in many schools outreach events during the period. The principal events include a stand at Southampton Science and Engineering Festival (March); 'Hands-on diffraction' with sixth form students (July); 'Science All Around Us' – activities for students from 10 primary schools (July); 'Into University' a year 6/7 workshop (August). There were also two significant events that reached out to the general public – An interview with the Director about the NCS on 'That's Solent' TV channel (September) and the Director involved in leading the Pint of Science 'From Galaxies to Atoms' event in Southampton (May).

### Facility staff training and career development.

Graham Tizzard and Sarah Milsted have assumed the roles of Operations Manager and Service Support Manager respectively as a result of restructuring the NCS with the new tender. These positions of increased responsibility have resulted in gaining significant experience in day-to-day, as well as strategic, management of the facility. Graham Tizzard holds the post of Outreach Officer on the BCA Chemical Crystallography Group committee. Sarah Milsted is managing BCA Outreach Bursary projects (vide supra). Peter Horton has taken on responsibility for all training and has conducted most of these activities. Wim Klooster was appointed and is progressing through probation well, in addition to further developing expertise in Charge Density Analysis. Gopikkaa Kanthasamy was appointed and progressed through probation and a range of training activities including the Intensive Crystallography School (Durham, March). Simon Coles has been appointed to the International Union of Crystallography CommDat committee and represented the UK at the IUCr General Assembly (Hyderabad, August).

**Commercial Service**

As of November 1<sup>st</sup> 2016, under a new tender, the NCS was able for the first time to deliver a commercial service to colleagues in industry. The first phase of delivering this was to port over established industrial interactions from the University of Southampton departmental service which performs regular work for large pharmaceutical companies as well as smaller (often local) industry. Accordingly, during the first half of 2017 this process began with the NCS assuming legal, financial and clerical oversight. Funding for a technician salary for 18 months had been found internally and a recruitment process conducted - Dr James Orton was appointed to the role of NCS Commercial Research Technician, which commenced in Sept 2017. The target is for this position to be financially self-sufficient by the end of 2018. This appointment enables any commercial work to be taken on without impacting on the other elements of NCS academic service delivery. The full commercial service commenced on 1<sup>st</sup> Sept 2017 (outside of this reporting period) and work billed for to date is around £5000.

In the feasibility study for this commercial activity an independent consultant performed some market research to establish that there was in fact an achievable market that was viable for the model of operation (where the facility itself was already fully funded). Further market research, now that the commercial service is proceeding, has generated a directory of potential clients. The new organisational model for the NCS has a 25% role for business development (both academic and commercial) – this is taken by Mrs Sarah Milsted and a plan is being drawn up for a marketing and engagement campaign to be conducted in 2018 to attract new business.

We are actively exploring new, additional models for commercialisation. The potential for NCS to form strategic business partnerships, as opposed to the “pay per structure” model, is strong – particularly if as part of a package with other University of Southampton capabilities. The Chemistry Department hosts Ron Swart of the Knowledge Centre for Materials Chemistry (KCMC, <http://materialschemistry.org.uk/>) and his role is specifically to link universities with industry – the NCS is working with Ron to develop these partnerships and projects.

**Additional funding received**

EPSRC Impact Acceleration Account funds have been secured to develop the Portal electronic management system (see Improvements section). This will be released as open source software for laboratory-based facility management upon completion. Whilst there are no current plans for NCS to financially exploit this thereafter, the efficiency gains and reduction in financial outlay for SME's as well as academia could have significant impact.

A modest amount of funding has been awarded by the BCA for development of Education and Outreach infrastructure and resources (see Impact – Training section).

A proposal to the Royal Society to support an African training network (coordinated by NCS) has been submitted. Proposals seeking funding to support academic projects with existing collaborators/users are being written with John Wallis (Leverhulme), Andrew Weller (EPSRC), Dan McAteer (DSTL), Robert Kingsford-Adaboh (GCRF), Sedat Ture (TUBITAK).

International Collaborations making use of the facility this period include: Franzisca Shoenebeck (Germany), William Zuercher (USA), Mohammed Nur-e-Alam (Saudi Arabia), Sabina Jhaumeer-Lauloo (Mauritius), Elias Vlieg (Holland), Krzysztof Wozniak (Poland), Srinivasulu Aitipamula (Singapore), Peter Turner (Australia) and several groups from Cagliari. Additionally to these, a selection of highlights include: Two separate, extended visits from colleagues in Turkey, Bunyemin Cosut (Gebze) and Sedat Ture (Bilecik), funded by travel grants from TUBITAK and both of which have generated collaboration and experimental results that will feed into future funding applications. Two PhD students from Wakayama Japan were fully funded (Grant-in-Aid for Scientific Research, Ministry of Education, Culture, Sports, Science and Technology, Japan) to work for 3 months in the facility. An international collaboration building on the radiation decay work (see Scientific Excellence section) has been established, where NCS will lead a team from Oxford, Aarhus, Bremen, San Francisco & Melbourne.

In February the NCS Director conducted a three day workshop at The University of Ghana (Legon) funded by the Royal Society and Department for International Development. This resulted in a strong collaboration with Prof Kingsford-Adaboh, the Dean of Science and a Government Science Advisor. A successful bid to host the Pan African Conference on Crystallography (Feb 2019) in Accra was submitted, resulting in Simon Coles being on both the steering and scientific committees. Building on this, a Royal Society/GCRF International Collaboration Grant to establish an African Crystallography Training Network and UK Exchange Programme was submitted by Simon which, if successful, will be coordinated by the NCS.

These collaborations have resulted in preparation or publication of 15 manuscripts and a highlight paper is “Novel solid forms of Ionidamine: crystal structures and physicochemical properties” *CrystEngComm*, 2017, 19, 2925-2935 (Aitipamula).

### Instrumentation upgrades

The most major instrumentation upgrade for the facility since 2011 was the installation of the new Hybrid Pixel detectors on two of the diffractometers (copper rotating anode and Ultra High Flux molybdenum rotating anode) during this period. This new type of X-ray detection is clearly going to be the next widespread step-change in crystallography and the NCS is amongst the first in the world to implement it outside of a synchrotron. Due to direct photon detection advantages are an order of magnitude faster data acquisition and no signal-to-noise background problems, meaning we collect better data, faster. We have been running these new detectors for over six months now and this is certainly the case, as we have seen a reduction in the number of samples requiring referral to Diamond and faster turnaround times for sample queues. The first article manuscripts containing data collected by these new detectors were being prepared for submission at the end of the reporting period.

A significant amount of the ancillary equipment around the diffractometers has also been repaired and/or upgraded as a result of renewal funding. The most significant of these is the installation of new cryogenic equipment on the copper rotating anode, equipped with a liquid nitrogen auto-fill which will improve laboratory efficiency and enable longer unsupervised data collections. We are refurbishing some of the replaced equipment to be used for emergency back-up.

### User Experience

The Portal on-line electronic access and management system continues to undergo incremental improvements, however we have recently embarked on a project that will increase its sustainability. EPSRC Impact Acceleration funds have been secured to redevelop Portal. This project will recode the entire system onto a more future-proof platform which will make the system considerably more extensible and maintainable. As a result a number of improvements will be made, with our goal to be for seamless management for facility and users alike from application all the way through to dissemination of results. A key element of this work is the identification of a generic “kernel” of code that would be the suitable basis for electronic management of any scientific facility. The goal of this latter piece of work is to produce and package a generic facility management system for exploitation both by HEIs and also industry – this would be openly available software.

A key component of the renewal tender was the introduction of a training programme, details of which provided are provided in the Impact section of this report. These initial courses have been a resounding success, with attendees providing topics for future events and indicating they would come again. These events are primarily for users of the NCS and this significantly improves the way they can analyse our data or interpret and exploit our results. However, we are also catering for the broader chemistry and crystallography communities and this has the benefit of increasing our visibility and ultimately increasing the number of users. We have also responded to user survey feedback and revised the format of the CIF results we generate and send to users, so that they are much better prepared for publication.

### Long Term Sustainability

Four Advanced Techniques will be offered with the first already on-stream and the others in a ramp-up phase. These will be pump-priming studies, aimed at performing exploratory work that will provide the basis for seeking independent funding that will leverage NCS facilities and expertise. The commercial service is initially concerned with providing fast and reliable single crystal structure analysis for industry. The first service to be offered is a “pay per sample” model, however the intention is that more strategic industry partnerships will be developed. The legal, financial and operational aspects of this service have been set up during this reporting period, with staffing and ramping up due to occur during the next.

The NCS fundamentally supports the EPSRC 2015 Strategic Plan and current Delivery Plan at the highest of levels by providing underpinning knowledge across the whole of Chemistry that informs other fields. As a world leading facility, it enables a broad portfolio of work that helps place the UK as a leading global research nation and feeds in to most aspects of the outcomes framework. The technique of crystallography and thereby the facility, transcends disciplinary boundaries and accordingly supports most elements of interdisciplinary research that touch on the chemical sciences. The NCS forms part of the 'National Capability' landscape by providing "support for excellent, long-term disciplinary and multidisciplinary research in engineering and the physical sciences."

Since the NRF Directors meeting in March 2017, we have been working on methods to gather more quantitative information on how the NCS supports EPSRC's strategic priorities. At that meeting an exercise was conducted around understanding the research areas that the NRFs support. Building on this, we have identified the Balancing Capability Research Areas supported and mapped them against the EPSRC Prosperity Outcomes. The first use of this mapping is now implemented as part of our application for access process, where applicants are now asked to self-identify which Balancing Capability Research Area(s) they work in. Accordingly, users have identified the work the NCS supports as being in the following areas:

Prosperity Outcome	Balancing Capability Research Area
Resilient Nation	Carbon capture and storage, Energy storage, Hydrogen and alternative energy vectors, Materials for energy applications, Solar technology
Healthy Nation	Chemical biology and biological chemistry
Productive Nation	Catalysis, Computational and theoretical chemistry, Synthetic coordination chemistry, Synthetic organic chemistry, Synthetic supramolecular chemistry, Analytical science, Chemical structure

A review of NCS marketing and user engagement strategy has recently been instigated. Future marketing and engagement will have an emphasis on new users in Balancing Capability Research Areas where the Strategic Focus Highlights are 'Access to research infrastructure' and/or 'Partnering with business'.