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Synthetic Methodology
Chemistry Innovation Position Paper 2009

Summary

The UK's position at the forefront of the pharmaceutical and fine chemicals industry is being challenged in the increasingly demanding global marketplace. To maintain its position the UK must ensure that it retains and continues to develop world class industrial and academic capability across the sector and specifically within the fields of catalysis and synthetic chemistry. Research must be fully integrated with world class process science and chemical engineering to allow successful research and innovations to be commercialised and fully exploited. Academia is integral in training the next generation of research scientists for both academia and industry and can contribute significantly to tackling the major synthetic chemistry problems faced by the process industries.

This consultation was undertaken to address the question: Why are academic chemists and funding bodies not more supportive of the challenges industry faces to overcome existing synthetic chemistry problems through the commercialisation and exploitation of novel solutions? There is a strong desire from both the industrial and academic synthetic chemistry communities to work well together and many productive collaborations already exist. The challenge is to improve the impact and value of such collaborations to produce commercially viable outcomes.

The output of any collaborative work is fundamentally shaped by the scope and type of funding mechanism which supports it. The funding landscape for collaborative applied synthetic chemistry is dominated by EPSRC CASE awards and TSB collaborative funding calls. Other funding streams include other EPSRC mechanisms, other RCs and routes such as European FP7 funding, but this is less significant in impact. Uptake of alternative routes such as KTPs and RDA innovation vouchers only represents a small proportion of spend/uptake. CASE awards were championed by the academic community and are seen as world class, whilst TSB calls were seen as effective, but less widely available and targeted in other areas.

Effective call definition is essential and if this is combined with succession funding for successful work a powerful solution results. Creativity in the definition and forming of funding calls was seen to be crucial and a clear route to this would be to have a much more involved working group consultation from conception to call definition. There must also be creativity in the call description whereby the call is made broad enough to be interesting and is not prescriptive.

One of the largest challenges is to incorporate process science and chemical engineering into the calls to provide tangible industrial solutions to synthetic problems. Such a multi-disciplinary approach would fit easily into TSB collaborative research call, but a change in focus would be required to successfully establish a multi-disciplinary CASE project through the use of multiple, linked CASE awards.

Very strong support was expressed for the CASE system which can produce world class results and training, but it was seen as being under threat and in need of reinvigoration. To maximise the impact of the CASE system continuation of funding mechanisms must be in place and exploitable. The under-utilised (in the chemistry-using sector) TSB Knowledge Transfer Partnership scheme (KTP) is one such avenue for funding.

This Position Paper highlights the role of Chemistry Innovation in tackling the synthetic methodology challenge and gives clear recommendations for the funding bodies, academia and industry.

Key Recommendations

Chemistry Innovation will:

- promote the importance of synthetic chemistry as an underpinning discipline
- help to facilitate challenge definitions that will define ideal project areas that are linked to societal and market issues
- seek to improve the delivery and management of applied synthetic chemistry projects
- enable follow-on work to successful projects through networking, knowledge transfer and further project support
- promote a continuum of funding mechanisms from small feasibility studies (e.g. RDA innovation vouchers) through CASE awards and KTP to commercial exploitation
- work with partners to support 'Introduction to Chemical Engineering for Chemists' courses and material

Industry should:

- understand academia's 'business model'
- should be open and clear about the what they do and don't want to see in a solution
- identify transformations that need to be improved (not reactions)
- seek to use KTPs to follow-on successful CASE projects

Academia should:

- understand industry's 'business model'
- recognise collaborative industry definitions of process chemistry problems as exciting challenges and targets for research
- develop efficient solutions to synthetic chemistry problems with straightforward work-ups
- seek to use KTPs to further successful PhD projects

Funding bodies should:

- provide fewer, more focussed calls
- recognise the importance and quality of the CASE system
- use the correct reviewers to understand the problems – industrialists should be used
- use part of their calls for high-impact, applied catalysis and synthesis research projects that can provide step-change improvements in process chemistry
- encourage a clear dialogue at the start of collaborative R&D projects to ensure the requirements are agreed and understood
- consider multidisciplinary projects for applied synthetic chemistry problems – e.g. chemical engineering involvement – this could perhaps be achieved through Doctoral Training Centres

Funding successful innovation: Synthetic chemistry (UK)

Vision & Aims

The UK's position at the forefront of the pharmaceutical and fine chemicals industry is being challenged in the increasingly demanding global marketplace. To maintain its position the UK must ensure that it retains and continues to develop world class industrial and academic capability across the sector and specifically within the fields of catalysis and synthetic chemistry. Research must be fully integrated with world class process science and chemical engineering to allow successful research and innovations to be commercialised and fully exploited. Academia is also integral in training the next generation of research scientists for both academia and industry.

Value of the Sector

Pharmaceuticals in the UK has an annual turnover of approximately £50 bn, making this sector one of the highest contributors to GDP. Fine chemicals manufacturing contributes a further £30 bn per annum to GDP and the two sectors are linked through the industrial supply chain. Improvements in the discovery, synthesis and manufacture of new chemical entities will typically deliver millions in benefit to companies, and feed into other chemistry-reliant sectors. A sustainable, innovative and competitive UK synthetic community is vital to these industries and a major factor in their global location.

Effective funding of high impact applied research

The purpose of this document is to convey the successes and limitations of the established UK funding processes for applied synthetic methodology research, together with a vision as to how this situation can be improved. The content described here was generated through a consultation workshop (June 09), which was facilitated by Chemistry Innovation and brought together key representatives from both academia and industry.

The current funding situation

The objective of industrially focused academic funding is to allow industry to exploit the significant academic strength in the UK to address important industrial challenges. In an ideal situation, industry gains novel or innovative solutions to its challenges, which it is able to commercialise, whilst academia gains high quality, industrially relevant results which are publishable in high impact journals. The research scientist involved also benefits from high quality training, which leaves them well placed for their future career. Companies gain from access to academic expertise and knowledge.

Funding routes

Within the synthetic chemistry sector the EPSRC and the Technology Strategy Board (TSB) are the two most important UK funding bodies. Other funding does exist through alternative Research Councils and funding bodies, particularly for multi-disciplinary work, but such funding mechanisms are analogous to those described here. European funding also exists through funding schemes such as Framework 7 and Marie Curie, but this will not be discussed within the scope of this document.

The EPSRC Industrial CASE awards are seen as a very strong funding approach, whereby businesses apply for and then award PhD studentships. In addition to this a number of key industrial partners are awarded a quota of CASE awards each year. The businesses take the lead in arranging projects with an academic partner of their choice. To increase the scope and impact of this work CASE awards are also awarded through agents such as Knowledge Transfer Networks (KTNs) and regional development agencies. The CASE students are expected to spend at least three months of a three and a half year award working at the supporting business.

The TSB has the objective of driving business innovation in the UK and one of its core approaches is the funding of *Collaborative research and development.* The TSB states that such funding is designed to assist the industrial and research communities to work together on R&D projects in strategically important areas of

science, engineering and technology, from which successful new products, processes and services can emerge. Practically the TSB issues calls in a strategically important area and a consortium of academics and industry is formed to meet these challenges.

Knowledge Transfer Partnerships (KTPs) are an alternative scheme managed by the TSB to enable companies to identify the most appropriate source for the knowledge or capability required to address a research challenge from within the UK's knowledge base (universities, colleges or research organisations). Within the chemistry-using sector KTPs primarily provide funding for a researcher, supported by a lead academic, to be embedded into the company to complete a high impact project. KTPs provide the mechanism to address new challenges or to take lead techniques and skills from academically based projects (such as CASE). KTPs typically last between 1 to 3 years, whilst the newer short KTPs last between 10 and 40 weeks. Industrial uptake of KTPs is low in the sector and awareness within the academic community is also low.

Delivering successful projects

In broad terms successful projects require a clear definition of the challenge, a consortium of the right people and the right level of resource to meet the challenge. Effective project management is also required across the life time of the project to ensure good interaction between the partners and that the milestones and project goals are met to the satisfaction of each member of the consortium.

As scientific research should be challenging there is inherent risk within any research project, but the right level of risk must be incorporated into the projects to enable step-change innovation and world class results to be delivered.

Chemistry Innovation is recognised as having a strong record in monitoring and supporting CASE projects through its annual allocation. Chemistry Innovation managers maintain contact with the project team throughout the duration and seek to ensure continuity where the collaboration is successful and requires follow-on project support through to exploitation. The benefits to the company are captured at the end of the project. The student is supported throughout via visits and attendance at Chemistry Innovation meetings. Chemistry Innovation can help in bringing additional partners to the project and in dissemination of the results.

The consultation

Whilst many successful examples of collaborative research projects exist, this consultation was undertaken to determine where improvements can be made throughout the process with a particular focus on applied research projects. Could the mechanism of setting up projects better enable tackling of major industrial synthetic chemistry problems?

The views described here are those of the participants – who were industry experts and academic leaders. The key issues are summarised below:

Maintaining chemistry's profile and funding

Historically chemistry has been well supported but in a very competitive funding environment the consensus of opinion is that its profile is dropping. Despite underpinning many funding themes chemistry is not a specific theme for either the EPSRC or TSB and is in danger of being overlooked.

Leveraging funding

- A compelling case must be made to government and funding bodies that chemistry and chemistry related issues are essential and provide value for money
- Synthesis must been seen as important and key to Grand Challenges.

Industrial CASE awards

- The strength of support for the CASE system was very strong across the board. This funding approach was judged to be highly effective and world class.
- There was a degree of frustration that such a strong system was being allowed to decline and it was seen as very important to reverse this. "....we had a system which was the envy of the world and now we are in danger of losing it."

Challenge definition

The key to successful, impactful projects is good challenge definition, which then allows the successful consortia or research grouping to tackle the important themes.

Successful challenge definition requires the definition of a challenge area followed by definition of the themes within the area. To make this relevant a period of consultation is required from high level interaction with steering groups and think tanks, to engagement with the knowledge experts and the implementers (industrialists).

Open consultation: Defining the challenge

- There is a very strong desire between both the academics and industrialists to collaborate for mutual benefit. There is an awareness that both groups often have different the aims, with the academics wanting to publish work close to their research interest and industry's desire to solve proprietary problems. These two aims are not mutually exclusive, but both partners must be clear about their required outputs.
- From an academic perspective openness (of the industrialists) was described as essential. "We need to know the *do nots* as well as the *dos!"*
- From the Industrial perspective, there is a recognition that academic work is very good, but that current academic output can be "all about the reaction" with the work-up seen as incidental. Industry requires effective routes with efficient or achievable work-ups
- All parties recognise that solutions to synthetic problems should be efficient and elegant. Speed to the best route is also very important. Challenges could also embrace and overcome the challenges raised by legislation.

Open consultation: Engaging all partners

The challenges must engage all the partners. Such engagement retains interest and leads to successful projects

- Both partners should understand each others' drivers and business models

- The academic desire is that the work must be publishable and funding calls must drive towards challenging publishable problems, whist industry requires solutions to often sensitive propriety problems, which can be readily commercialised
- A very strong message was that transformations, not reactions, should be identified. It was also desirable that funding calls were structure such that provide and reward "interesting" challenges.

It was recognised that the missing link with exploitation of a lot of the good results was in Process Science/Chemical engineering

Scope of the challenges: Exploitation of research

- It was seen as highly important that organic synthesis is exploited by linking it to chemical engineering via physical organic chemistry
- Rather than just funding chemistry research in isolation, funding of multidisciplinary projects with chemists and process scientists engaged on the same challenge was seen as essential. Multi-disciplinary projects involve several researchers with strong skills in their own areas, which is distinct from interdisciplinary projects, which require individual researchers to cover a range of areas which results in them typically developing a broader range of weaker skills

Barriers to multidisciplinary challenges

- There is currently poor physical integration between most chemistry and chemical engineering departments in the UK. This is not the case for key competitors such as the US
- There is a language and terminology barrier between the two disciplines, which is seen as a large potential problem

In theory neither of these barriers should be insurmountable but there needs to be an emphasis on collaborative work

<u>Key outputs</u>

Generation and exploitation of ideas and IP

- Innovative ideas and solutions are core to the success of industry
- Industry's needs must be understood (e.g. pharma) to determine where profit will be made in the future. There is a need to focus on today's problems and identify solutions, through approaches such as new reactions
- High quality, publishable academic work

Development & retention superior talent

- Chemistry must be promoted to ensure that the best students study chemistry
- The quality of UK student training must be high & drive creativity
- The brightest students & post docs must be retained in the UK, although this can only be achieved by high levels of funding and opportunity

Recommendations

Maintaining chemistry's profile and funding

High quality research and innovation should sell itself, but one of the key roles of Chemistry Innovation is to continue to lobby funding bodies and government to ensure that the values of chemistry is continued to be understood

Challenge definition

World class challenge definition requires the right level of consultation with the right people and strong decision making. The traditional autocratic approach of consultation, followed by decision making in isolation has its merits, but there is space for innovation in the approach which is used.

Challenge definition may benefit from a more iterative approach, such as using a working group involving academics & industrialists, which is able to take the challenge from ideas stage to proposal. This would help to clarify the challenges & specific requirements. It would also ensure that the challenges are written in the right language.

It is stating the obvious to say that the best way to maximise the impact of challenges is to be able to focus a high level of resource in key areas. The difficulty is always to define the right areas and to give the right amount of autonomy or steer to the research. There was a strong feeling that more focus of the work was often needed to cluster effort in the right area. It was proposed that a "series of challenge questions should be developed that define ideal project areas".

Whilst TSB collaborative funding lends itself to the funding of consortia with multiple partners there was a strong view that, often by nature of its definition: one problem defined by a single company and addressed by one student typically with only one academic supervisor, much of the CASE research was completed in isolation. It was seen that if multiple CASE awards were clustered then their impact could be much higher and more valuable. A good example of this would be the funding of multi-disciplinary projects, whereby chemists and engineers or process scientists were co-funded on the same projects. Such an approach, particularly if both students were co-located, would bridge the gap between the two disciplines and give a very strong project output.

Bridging the Chemistry and Chemical engineering gap is not, however, trivial and a concerted effort is required to achieve this. Some interaction does occur, but further forums and seminars must be established to bridge the terminology gap and to enable both parties to talk a common language. More fundamentally important aspects of the underlying science must be taught and understood, through courses such as RSC's "Chemical Engineering for Chemists". Such courses should be focused on the science, such as mass and heat transfer, and not the equipment.

The decision process: Review of funding proposals

Applicants for funding always benefit from a good level of feedback on funding proposals, particularly if those proposals are unsuccessful. It is also essential that the reviewers are of a high calibre, with the right background and experience. The suggestion was made that the Research Councils, such as the EPSRC, must ensure that they choose the right proposal reviewers who understand the problems and that industrialists could be used in conjunction with academics.

Exploitation of work: maximisation of impact

Continuation funding of successful work is highly desirable for all parties involved. This is particularly important if strong progress has been made but further work is still required to overcome the remaining challenges and open the way for exploitation and commercialisation.

The situation was succinctly summarised:
"Expectation must be managed: With enabling (longer term) challenges don't expect academics to produce the finished article"

To make/emphasise the point it was highlighted that:
"...it is necessary to break the EPSRC cycle which involves 3 years funding and then starting again"

The value of KTPs in this situation cannot be understated. This funding is ideally positioned to allow the original student, or Post Doc group member, to become embedded in the sponsoring company and to progress the work with the support of the academic and university expertise. A pivotal role of Chemistry Innovation is raise awareness of this and to facilitate the application process. After a lack of awareness of the programme, there are two main obstacles for KTP uptake. The first is the level of detail which is required in the researcher's workplan and the perceived level of inconvenience this represents. A rework of the KTP funding form for scientific research: definition of the aims of the work programme and top-line detail of the implementation, would quickly address this. The second obstacle is the low value to which some academics perceive that they receive from their investment of time. If KTP participation was recognised by the funding councils through future research funding, this would become more appealing.

The enthusiasm of a wide proportion of the academic community to engage with industry is very real and cannot be overstated. The role that KTPs, or similar Research Council funding, could play was emphasised by the unprompted strong support for a flexible or responsive CASE-style funding to allow industry and academia to collaborate. It was suggested that industrial secondments for academic chemists in key areas of interest would be highly beneficial and debate ensured over the ideal length of these secondments: 2-3 months or 6-12 months.

Conclusions

The industrial and academic synthetic chemistry community are already well engaged and frequently collaborate with each other. Creativity in the definition and forming of funding calls could be very impactful and one route to this would be to have a much more involved working group consultation from conception to call definition. There must also be creativity in the call description whereby the call is made broad enough to be interesting and is not prescriptive. For example this could mean that transformations to solve problems, not reactions, are described in calls.

One of the largest challenges is to incorporate process science and chemical engineering into the calls to provide tangible industrial solutions to synthetic problems. Such a multi-disciplinary approach would fit easily into TSB collaborative research call, but a change in focus would be required to successfully establish a multi-disciplinary CASE project through the award multiple, linked CASE awards.

Limited feedback was given on TSB funded projects, but very strong support was present for the CASE system, which was seen as being under threat and in need of reinvigoration. It should be stressed that CASE awards are seen to be world class and the envy of many other countries. Crucially one of the weakness of the CASE system has been that a significant amount of work is not progressed through lack of continuation funding. It is vital the additional funding is available for encouraging work to allow it to be fully exploited and this could be done either through establishing an additional EPSRC funding stream or through fully utilising the underused TSB KTP funding. KTP funding is a very good fit for this approach, although it could be reviewed for research science as small changes in the application form would dramatically improve its uptake. Chemistry Innovation is well suited to promoting KTP and this is central to its role.