Title: Review of "Centro de Química – Vila Real".

The "Centro de Química – Vila Real" (CQV) is a research unit belonging to the Department of Chemistry at the Universidade de Trás-os-Montes e Alto Douro. The center consists of 28 Ph.D researchers, who work in the areas of a) Organic Chemistry, Natural Products and Food Chemistry, b) Materials Chemistry and c) Environmental Chemistry. The main objectives of the CQVR are to conduct fundamental research in the area of Chemistry, promote education for students interested in a research career, serve the scientific community, foster interdisciplinary work through collaborative projects and collaborate with outside institutions in research activities.

For the purpose of this review, the peer group that I am considering is Research Units in Chemistry across Europe and the USA. With this premise in mind, I have addressed in this review the following issues:

Quality and quantity of the research performed at the facility in terms of research publications, and other outputs.

The quality and quantity of research performed at the center is very good. The research topics are of great scientific interest, and the application of various techniques to solve these problems is well thought. I particularly like the fundamental scientific approach conducted by the center. This combination of strengths is evident in the good number of scientific publications and grants awarded. However, to further assess the impact of the CQVR, it is important to describe the number of invited lectures/talks given by the center's faculty.

Research Themes

The research areas described by the various research groups are very specific and in my view not appealing to the general chemistry student. This is turn affects the number of students enrolling in chemistry research. Therefore, my recommendation is for the research groups to list thrust areas, which represent general areas of research as for example: a) Alternative energies (solar, fuel cells, batteries, etc), b) Water pollution, c) Pharmaceuticals. Subsequently, each faculty member can describe in more detail their own research interests within the general thrust areas.

Accountability

As mentioned above the quality of the research work and scientific staff is very good. However, it is very difficult to assess from the list of publications who is the Principal Investigator (PI) and who does what. Invariably, the papers have many authors and the author's order in a particular publication seem rather random. In this fashion, it is challenging to determine the leader of the project, which in turn decreases visibility for the center. My recommendation is to

1) Reduce the number of authors to a minimum, provided the research is not compromised and the quality is maintained.
2) Always list the PI as the last author of the paper. If there is more than one PI, the group should decide who should be the leader of the project.
3) On the webpage of each PI, define very clearly who are the postdocs, Ph.D students and undergraduate students working on the PI's group, so that the readers of the papers can relate the names of the authors with their function in the group. In addition, specify the PI for a specific grant.

Overall Impact of the center

At the moment, the CQVR already lists several items, which help assess the performance of the center, such as the number of Ph.Ds graduated, number of publications, Patents, Oral presentations and books or book chapters published. In addition to these, I recommend the following: number of papers per Ph.D student, number of citations per paper, funds raised per Ph.D student, invited lectures/talks and the current work location of the Ph.D, Masters and undergraduate students that have graduated.

The purpose of a research center, such as the CQVR is to be able to bring a significant number of researchers and resources to provide a synergetic effect. In this regard, it is important to relieve the PI, responsible for preparing a large proposal, from teaching duties during a period of time. Writing such large grants is very time consuming and requires focus, which is challenging if the faculty has to be involved in many hours of teaching.

Lastly, having in mind the geographical location of the CQVR, with respect to the decision centers in Lisbon, I would recommend placing a liason from the University of Tras-os-Montes in Lisbon or planning regular visits to the main agencies to get better acquainted with the decision processes.

Summary Statement

In summary, this reviewer feels that the CQV is performing very good research and offers expertise and instrumentation in various areas. However, at the moment, this work should be given better national and international visibility. In order to do this, the CQV must clear state the thrust areas of research, define the number and order of authors in the publications, increase the number invited lectures/talks, reduce the teaching load of PIs working on large research proposals for the center, assess the overall impact of the center and finally be better positioned with respect to the centers of decision in Lisbon.

Austin, November 21, 2010

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UTAD CHEMISTRY RESEARCH CENTER

Review on the Environmental Chemistry Research Group

This review is based on the contents of several documents: annual reports, FCT assessment and on a visit that took place last 28 January with a programme that included presentations of the Center and of the Research Group resources and activity, discussion and visit to the labs.

It covers the year 2010 and is organized in the following chapters: resources, outcomes and conclusions & suggestions.

Resources

1 – Permanent Staff and Students

Permanent staff has 9 members, 7 of them being career university professors and thus only dedicating around 50% of their time to research. During the visit I could verify their high engagement and enthusiasm. The technical background of these members is quite diverse which may constitute an advantage provided their competencies are combined in research projects, which already happens here and there. On the other hand this diversity may put some threat to the stability and cohesion of this research group, if the usually present "centrifugal" forces are not kept to the right level.

Also technical staff is reduced to a minimum which may cause problems to the correct and productive operation of heavier equipment.

Non-permanent research staff has about 20 members, most of them undergraduate and master students and 2 PhD students. The number of PhD students is small, much less than 1 per permanent staff FTE, thus there should be an effort to enroll more PhD students and to find means to support them.

2 – Laboratories and Equipment

Laboratory space is becoming scarce for the actual level of activities and part of it deserves renewal .

Some new equipment recently obtained through specific funding is already operational but, as reported, other heavier equipment is still necessary both for substitution of older existent equipment and to match new research needs.

3 – Financial sources

The research group has been able to succeed in finding money to support their activity from different national funding agencies like FCT, AdI or regional funds like ON.2. One important aspect that should be underlined is the research group ability to make research and services contracts with companies. Nevertheless it is important to think in diversifying and simultaneously internationalizing financial sources for example by submitting projects to EU, NATO, bilateral research protocols, etc.

4 – Other

UTAD provides for library and general informatics at a level that may be considered adequate.

Outcomes

1 – Publications

The level of publications in international journals (43 in the period 2007-2010, around 2/FTE) is good and the group managed to publish in some reference journals of its area.

2 – PhD & MSc

During the period from 2007-2010 12 MSc and 3 PhD were concluded. The number of PhD concluded is small because the number of PhD students enrolled is also small.

3 – Technology Transfer

The group has an excellent record both in patents (11 in the period 2007-2010), pilot plants (2) and services to companies.

Conclusions & Suggestions

This research group operates in the following sub-areas:

1 - Application of Advanced Oxidation Processes
2 - Biological treatment of industrial wastewaters
3 - Valorization of agro-industrial by-products
4 - Interaction of humic substances with organic and inorganic contaminants
5 - Organic matter, C and N cycling in soils
6 - Animal manures: P bioavailability and site vulnerability to P losses
7 - Hydrogeochemistry and geomathematics

These sub-areas reflect the different origins and competencies of the permanent research staff which is an asset to do research and development in the environmental chemistry area in itself a transversal one.

The group members are relatively young and profoundly engaged .

Physical and financial resources are at a level that can support present activity but will become scarce if the activity level increases, which I think is and should be the desire of the Group members, of the Research Center and of the University.

The group has a good average rate of publications in SCI journals and is quite strong in technology transfer, so in developing technology from fundamental research results, which is a unique and distinctive feature that should be kept.

The group has been able to find sources to finance its activities, where a non-negligible part comes from projects with and services to companies.

Last FCT assessment rated the Center with a Very Good mark, certainly with an also very good contribution from this group.

Naturally the Research Center targets a mark of Excellent in the future.

This Environmental Chemistry Research Group should contribute to that goal. For that I have the following suggestions:

- Increase the number of PhD enrolled;
- Increase the international cooperation;
- Try to increase and improve technical support;
- Improve physical space and find financing to more equipment;
- Diversify the financing sources by applying to foreign agencies,

in order to:

- Increase SCI journals publication rate;
- Maintain the level and quality of technology transfer (patents, prototypes, pilot plants, services);
- Increase the number of PhD concluded;
- Maintain or improve outreach activities.

February 22, 2011

(Carlos A.V. Costa)

Review of Organic Chemistry, Natural Product and Food Chemistry Group

This report reviews the activities undertaken by the Organic Chemistry, Natural Product and Food Chemistry group of the Centro de Química – Vila Real, Universidade de Trás-os-Montes e Alto Douro, for the year ending December 2010 (Date of visit 18th- 20th January, 2011). Key sections of activity have been identified and a commentary on each is presented with good practice and weaknesses (with suggested remedial comments) identified. The summary indicates the current level of the group's performance.

Staff

The section is composed of eleven enthusiastic academic (PhD) permanent staff members, all of which contribute the core activities of research, teaching and administration of the group. The average age of the staff is *c*a. 44 years and, whilst young, the university should begin to consider the infusion of 'new blood' in the near future to either establish a new research theme or bolster one of the current activities and assist with the generally high teaching and administration workloads. An alternative approach makes use of visiting professorships, who can make valuable short term contributions to specialist teaching and research activities.

Research

The academic staff conduct both fundamental and applied collaborative research into two main themes, Functional Dyes and Biologically Active Compounds with the former subdivided into cyanine dyes and photochromic systems and the latter into food chemistry and natural products. These research themes are worthy of investigation considering, for example, the impact on health and nutrition of food chemistry, and the resurgence of interest in functional dye chemistry with new applications in solar energy conversion, sensors and fluorescent imaging and medicinal dyes.

Publications

The group does a very good job of disseminating their research results through publication in a wide variety of leading and specialist journals and both the number of publications and the impact factor of the journals selected are showing an upward trend over those of the previous year. However staff should engage a research strategy to target their submissions towoards the

very highest quality journals (impact factor, citations) in the first instance. A further strategy would involve the submission of topical review articles to leading journals as a means of increasing the awareness of the wider scientific community to the research activities at UTAD.

The group where possible should continue to generate and protect their intellectual property with patents but should, where permissible, follow these up with full academic papers, thus increasing the impact of their activities.

It would also be useful to evaluating bodies for staff to include data on conference organisation and attendance/presentations at major conferences – perhaps the web pages (see later comment) would be useful to display this information.

Research Income

Academic staff have been successful in attracting very good levels of research funding, for example, from the FCT (functional dyes) and industry/QREN (food chemistry), given the amount of time that it takes to generate good applications and the frequency of calls from funding agencies. The presence of 'partner' industrial funding is very desirable and staff are encouraged to engage as widely as possible with industry. Collaboration with other national research groups in funding applications was also evident though often the group was a smaller partner.

A notable absence in the grant portfolio is evidence of applications to the European Funding Agencies (FP7 programme). This deficiency should be addressed, especially in the current climate of global recession where national support may become harder to secure. For staff to be successful with large FP7 applications, which are lengthy and administratively complex, they require administrative support and intelligence (from a central University funded research office) and quality research time. Could a rotating sabbatical system be employed to assist the lead applicants?

External Relations

The group web site is adequate but requires some attention to bring the content up-to-date (new images, most current publications with perhaps narrative on one key publication and a common style to individual web pages); the importance of the WWW should not be underestimated as it often provides the first point of contact with potential students, researchers and industrialists.

The group is commended for their outreach activities with regional schools but they should not become complacent, if possible more events showcasing some of the interesting research could be directed towards potential degree course entrants (tell and sell).

Opportunities exist to engage with national and international industrialists and key policy makers within funding organisations through invitations to present lectures and seminars within the department.

Facilities and Equipment

Quality space is at a premium in the shared main building and efficient (re-)organisation is essential if the group are to fulfil their ambitions. Laboratory space is somewhat dated though serviceable and a rolling programme of refurbishment should at least be planned by the university for such a time when finance becomes available. Where possible additional funds should be made available from the university and from grants and contracts (where such elements maybe claimed).

The group has had some recent successes in securing funding for equipment and have further bold plans for new items which need to be prioritised. A high field NMR instrument (300 or 400 MHz) would be of immediate use to those engaged in synthetic organic chemistry enabling more rapid progress. Additional items include HPLC/mass spectrometer, thermal analysis equipment and an elemental (CHN) analyser. However, routine running costs and maintenance must be carefully weighed prior to purchase, though with good management and entrepreneurial skills a small analytical service could be established as a secondary income source.

Science departments rely upon skilled technicians and with an increased instrument base comes the need for further technical support. Where possible technical support (technician hours) should be claimed on larger grants.

Teaching and Administration

The staff have, on average, *ca*. 10 formal contact hours per week with further teaching and financial (grant) administration duties. This is a very high load for research active academics and options (such as inclusion of teaching and demonstrating hours in PhD (training element) and post-doctoral contracts, new appointments, administrative assistance and effective timetabling) must be fully examined to reduce this to a more reasonable level.

The courses delivered encompass 1st, 2nd and 3rd cycle activities in food chemistry and biological subjects and a new 2nd cycle biochemistry course and 3rd cycle chemical and biochemical

sciences programmes are planned to commence in 2011. However the lack of a well-defined chemistry course is a concern as this provides a major source of PhD students. The staff are encouraged to examine more attractive subject options such as medicinal chemistry and chemistry major courses 'chemistry with ……..' and joint chemistry programmes. A regional activity focussed course on agro-chemistry may also be worthy of consideration.

Summary

Overall the Organic Chemistry, Natural Product and Food Chemistry group are performing at a high level in both research and teaching activities. Research output and income are very good and are improving and with some additional resource (staff, equipment, facilities) the group will push their very good research rating further towards the excellent category boundary.

A grading of VERY GOOD is recommended for the activities undertaken by this grouping for the period ending December 2010.

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