

## **GLOBAL REPORT ON THE EVALUATION OF THE RESEARCH UNITS ON CHEMISTRY**

Panel composition:

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The program of the 10-day assessment exercise, March 16-25, 2003, had been organized by the FCT following discussions with the coordinator. It was always followed very strictly, but for the changes described below in detail. The excellent welcome offered to the panel in all the units visited without a single exception should be stressed. The organization of the visits was largely left to the local unit coordinator as it was felt that the experience of the two previous visits would provide enough guidance. In general, an initial (short) presentation of the unit was followed by informal discussions between panel members and individual researchers in their laboratories and, in some cases, near posters that had been put up for this. The panel members asked frequent questions to clarify the unit reports or the presentations of the researchers.

The reports on the individual units were the results of contributions by panel members (from their appreciation of the units reports and from their notes taken at the time of the visits) and a thorough discussion in a meeting on March 25<sup>th</sup>. The panel evaluation and the marks and recommendations were gotten to by consensus. The coordinator was always available to help in the discussions and to clarify doubts about Portuguese research organization but made it clear that the final results were the responsibility of the foreign panel members.

As stated above, the schedule was followed but for the visit to Units #70 and #313 in Coimbra. As this implied important changes, the facts should be described here in some detail. Unit #313 had made it known informally to the coordinator of the panel and to FCT

that several senior members of the Unit might be called to give testimony in court on March 19<sup>th</sup> and requested another date for the site visit. After careful study of the schedule, the coordinator promised that, if the impossibility was confirmed by the court appearances, he would try to find an opportunity to go to Coimbra for a short visit at another occasion, perhaps on March, 25<sup>th</sup> in the morning. The only alternative would be asking some leading members of the unit to come to Lisbon to meet the panel in the closing day. However, this would depend on the progress of the panel work along the visits, as this last day had been reserved for a final discussion and for the preparation of the reports. As the visit to the other units in Coimbra would go ahead in any case, the coordinator of Unit #313 was asked and agreed to make a last minute effort to see whether the visit on the afternoon of March, 19<sup>th</sup> would be possible and call the coordinator's mobile phone at any time. On the 18<sup>th</sup>, the panel coordinator was told that the unit would not be available for the site visit and the possibility of the alternative special visit on March 25<sup>th</sup> was considered. As planned the panel visited two of the three units in Coimbra, #61 and #70 on March 19<sup>th</sup>. In unit #70, some members were not available so that the presentation went ahead but the dissatisfaction of the coordinator was clear.

By then, it was clear that the preparation of the final reports would be a lengthy process that would require a full day of work. Travelling to Coimbra in the morning of March 25<sup>th</sup> to visit unit #313 would not allow the panel to start working in the reports before 3pm, too late to complete the work required. The members of the panel had their flights set and staying another day was clearly impossible. Furthermore, the panel was not satisfied with the conditions of the visit to unit #70. The panel decided unanimously that the only way out was to re-schedule the program for Friday, March 21<sup>st</sup>, anticipating the visit to unit #62 in Aveiro and creating a slot of 1h30 for unit #313 and another slot of 1h for unit 70. On the evening of March 20<sup>th</sup>, the coordinator of the panel contacted by mobile phone the coordinator of unit #313 and asked him to arrange this change of program. After consulting colleagues, he kindly agreed not being sure, however, that all relevant unit members would be there, as they would be warned only by Friday morning. As the assessment of the teaching program on Chemistry (Licenciatura) was running concurrently, most staff members should be there and the visit was set to start at 17h00 to allow for the conclusion of that assessment. Accordingly, unit #313 was visited between 17h00 and 18h30 and unit #70 between 18h30 and 19h00. The organization of these visits was left to the decision of the unit's coordinators. Shortly after 19h00, the panel rushed to the airport of Porto to fly to Madeira, skipping dinner.

**#8#**

This is a unit with some interesting work in progress, with reasonable prospects of success, and an adequate though by no means outstanding record of publications in appropriate journals and of training of young researchers, both at Master's and at Doctor's level.

The most obvious criticism is the lack of any contact at all with the industrial concerns most likely to find applications for the work being done. On being questioned about this, at least three members of the unit independently gave essentially the same reply, that in Portugal there was almost no pharmaceutical industry, that such companies that exist are not interested in developing new products derived from original research done in Portugal, and that as individuals the researchers were more concerned with benefiting humanity than in purely commercial aspects. All of this may be true, and the last point may even be laudable, but it is questionable how realistic it is in a research unit devoted to specific and experimentally testable remedies for specific diseases. A different view might be possible in research on the general principles of drug discovery, but the unit in question is very clearly concerned with practical and experimental problems, and it is difficult to see how it can ultimately benefit humanity if it remains totally divorced from the world of commerce.

In summary, therefore, the unit should be strongly encouraged to explore the possibility of establishing formal links with the pharmaceutical industry. If it is not possible to do this with Portuguese companies there ought at least to be companies in Switzerland and elsewhere who could be expected to take an interest in the work being done, both in the novel ideas that are being developed in the unit, and in the specialist knowledge that some of its members have in the traditional plant remedies used in Guinea-Bissau.

With an appropriate technical environment (a new high field NMR machine will be available soon to be shared with the Faculty of Sciences) and with appropriate structural funding, this unit may aim at a level notoriety that it did not yet achieve due to the lack of application of its research projects. Too many lines of research remain at a preliminary level. Among the most advanced topics, the following may be registered:

- **Phytochemistry:** The study of plants endemic in Portugal and certain African plants, in collaboration with several international groups. Certain new compounds have been isolated and characterized. The group should now consider the in depth study of their therapeutic applications and its independence from international groups, especially when the new NMR machine becomes available. However, it should be kept in mind that international competition is tough in this area with certain groups where analysis and

screening are now automatic. Further to classical studies, it may be necessary to select some active molecules and make an advanced study of the mechanism and to develop analogues in a strategy of structure-activity relation.

- Drug design: The use of this term is not justified. Current studies remain at the level of a therapeutic study where researchers synthesise prodrug molecules without an explicit study of the structure-activity relation. Certain lines appear to be promising, e.g. the enzyme  $\beta$ -lactam inhibitors or the synthesis of analogues of tacrine.
- Toxicology: The main topics concern the risk of exposure to hexane and to mercury derivatives, for which many studies have been published. The originality of the project is not clear.

The group should consider the redefinition of their aims, making sure that their research topics are well justified and their originality is better assured.

#### **#61#**

The low level of funding provided to this unit after the previous evaluation was to some degree a self-inflicted wound, as it followed from their organizational failure to prepare adequately for the evaluation, with the result that work that would have contributed very favourably to the recommendation could not be taken into account because it was not published in time. However self-inflicted or not, the quality of work in the unit deserved better. It is fair, therefore, to say that all of the matters that gave concern to the 1999 panel have been dealt with more than adequately since then. The level of publication in appropriate journals is high, and it is no longer true to complain that biochemical work is published in journals unlikely to be read by biochemists.

Not only is the general standard of the unit high, but it is also important to note some new themes that are being pursued with vigour and success, and are likely to lead to significant improvements in medical practice. The methods of diagnosis being developed by Drs Jones and Carvalho are original in conception, simple and (reasonably) cheap to apply, and likely to be effective in a practical clinical environment. There is no reason why they should not be adopted on a short time scale for use in hospitals. This work forms part of a broader project in the use of NMR to study metabolism, which is comparable in quality with the best current work in this field.

Studies of lithium (in relation to manic depression) and vanadium derivatives (as potential insulin-mimetic drugs that could provide a cheap oral alternative to insulin for treating type I

diabetes) are being carried out. These are likewise of a good international standard and the vanadium derivatives have considerable potential value as medicines.

The Unit leader has an active imaginative research program with international visibility and international collaboration. Some of the younger members of the unit have developed interesting, novel research programs related to biomedical applications of NMR and which address problems of considerable interest. A point to consider is the possibility of collaboration with some organic chemistry teams.

A programmatic funding of Euro 124 640 is proposed to maintain and update the sophisticated and intensively used equipment that is available to the unit. If it were found to be crucial, a technician might be taken in.

### **#62#**

This unit gives a high impression of efficiency and homogeneity. Taking advantage of high-level technical resources, researchers can perform original and efficient chemistry in three different areas:

- Organic Chemistry, Natural Products and Catalysis
- Mass Spectrometry
- Food Chemistry

This appeared to be the best equipped in terms of Spectroscopic services of any of the departments visited during the evaluation exercise. There were 2 NMR's (300 and 500 MHz) and a high resolution mass spectrometer as well as a Q-ToF available to serve the needs of the synthetic chemists.

The different groups have a high level of publications with different IF reflecting the differences among the journals they send their articles to, but all of them publishing in the best journals of their disciplines.

The most relevant results in organic synthesis are the following:

- Synthesis of porphyrins and metalloporphyrins: an original subject with interesting results. New derivatives such as porphyrins coupled with sugar moieties and amino acids could find applications in therapeutic studies. Some others could be used as catalysts for oxidative transformations or photochemical studies.
- Synthesis of fullerenes : this project seems to be unique in Portugal. Interesting results are expected in a near future.

- Synthesis of various heterocyclic compounds: a classical chemistry is applied to prepare compounds of various interest, finding applications mainly in biological studies.

- Members of the Mass Spectrometry group also carry out research on a number of problems for which MS is the main research tool. Research projects are concentrated on the use of electrospray to generate metal complexes and biological species of high molecular weight. It was not possible to evaluate the degree to which any of the problems addresses had resulted in significant fundamental insights being developed.

For all these projects, it would be very important to be able to give information about applications for the next evaluation. The concept of "potentially interesting for applications" has to lead to real applications.

The mass spectrometry group appears to be very productive especially in collaboration with other groups.

The group devoted to food chemistry and led by Dr. I. Delgadillo presents interesting results. Most of the topics have been established in collaboration with local industries, especially those of wine and olive oil production. However it is not clear that a lot of new results were obtained, when compared to the last evaluation.

A programmatic funding of Euro 175 275 is recommended to upgrade some of the equipment identified as bottlenecks in the planed research activities.

### **#70#**

It is sad and disappointing that the problems that were evident with the relations with unit 313 at the time of the 1999 evaluation have still not been fully resolved. The presentation by Professor Amorim was in consequence much less persuasive of the quality of the unit than it probably could have been in happier circumstances.

However, it must be added that the subsequent presentation of the part of the unit devoted to educational research was little short of a disaster. The main conclusion that could be drawn from it is that the speaker is concerned neither with chemistry nor with research, and it is not at all easy to see any valid reason why she should be working in a unit of research in chemistry. The manner of presentation was that of a political manifesto and not a research report, as no results from any research (even research in educational methods) were mentioned, and the views expressed appeared to be outmoded and out of touch with modern studies of education. However, even if the work were of good quality there would be no reason to do it in a unit of research in chemistry. As it stands, retaining this theme

can do nothing but damage to the quality of the unit as a whole. This post-modern approach to social science research involved advancement of an exceedingly vague hypothesis concerning learning of science by high school students and then anecdotal accounts of its application. No statistical data were obtained to ascertain the efficacy of the approach and no learning outcomes or objectives were defined. The presentations were followed by a visit to the Raman laboratory of the Molecular Structure group. One of the spectrometers was functioning while the other was not due to a power supply problem.

The unit was visited a second time, as some members had not been able to be present on the first occasion. Unfortunately this second visit did little to improve the picture given by the first. The work on anti-cancer drugs appears to be driven more by wishful thinking than by a coherent research plan, and its representatives appeared unable to provide any convincing account of why they thought their approach would be likely to lead to valuable new drugs. The work on hydrogen bonds is of a higher standard, but the researcher mainly concerned with this has now moved to Aveiro.

There is clearly a problem with this Unit. The researchers appear to give little importance to the evaluation exercise. There was no enthusiasm nor clarity in the presentations. It appears to suffer from a lack of research students (no PhD thesis submitted in 1999-2000) and lack of technical staff. Still, there is some progress in scientific production. Among the research topics presented, the one concerned with platinum diamines lacks depth. The title appears to refer to a drug design rationalization on the synthesis of biologically active molecules or then it is medicinal chemistry as it was done in decades past when the preparation of derivatives of a biologically active molecule was sought for no other reason than the availability of the reagent.

#### **# 81#**

This Unit has 33 PhD staff and produces quite a number of publications and also theses. They also have many international collaborations. The major input is from the thermochemistry group, Line 5, and especially, Aníbal Varejão Ribeiro da Silva (31 papers). The productivity of the other members of the Unit is not exceptional. The message that was sent in the previous evaluation has not been heard. Unfortunately the documentation received is not up to date and poorly organised.

One great success has been a Patent application by members of the Analytical / Food group (diacetyl in beer). This has led to close collaboration with the brewery and the members of the Unit are very pleased with that.

Group 1 “Organic Synthesis of Bioactive Compounds” is a new group created two years ago; some promising results have been already obtained in two areas of research : peptide chemistry and nucleosides analogues. Some applications to the preparation of anti-malarial and antimicrobial peptides seem to be interesting. The idea is to prepare some pro-drugs that would undergo hydrolysis in the blood stream increasing bioavailability. The size of the peptides prepared in this group is in accordance with the possible analytical studies encountered in the group.

The activity of Group 2 “Free radical and Food chemistry” is mainly devoted to the study of components of wines and olive oil. Polyphenolic have been isolated and characterized. Their interaction with proteins of saliva is now studied. Concerning aroma compounds from oil, researchers are now studying their interaction with cell membranes. Some original results might be obtained in a very near future. It will be very interesting to follow these results for the next evaluation. A strong collaboration with a French group can open new perspectives to these projects.

Group 3 “Analytical and Coordination Chemistry” followed the recommendations of the last evaluation concerning the application of their research on analysis of diacetyl in beer. A patent has been applied which could led to relevant applications in European breweries. New studies on the determination of other components are in progress. This group is acquiring a solid knowledge in this field which has to be supported.

One potentially very interesting project is that of Anna Martins in Group 4: enantioselective oxidation of glucose (D- / L-) on gold surfaces; these were specially prepared but not using optically active template.

The leader of group 5, Professor Ribeiro da Silva, has a long-standing reputation in the area of Thermochemistry. The quality and quantity of the thermochemical data generated in his laboratory has been truly remarkable and, as calorimetry laboratories in other countries have closed, Portugal has become the best source world wide of such data. The techniques used, although classical in origin, have been up-dated with modern electronics and new technologies as well as being computer controlled. This has dramatically increased the accuracy and precision of the data generated. Within the group there are a number of investigators, each of whom has taken over a particular specialization within the field of thermochemistry. For example, there are teams in combustion calorimetry, vapour pressure measurements, thermochemistry of metal complexes, solution reaction calorimetry and microcalorimetry. More recently a program was initiated in electronic structure calculations to complement the experimental data.



The site visit left a very good impression. Overall, the younger chemists in this unit are extremely enthusiastic and competent. The final rating proposed should be seen as an incentive to the full unfolding of the group capabilities in the near future.

To accelerate the establishment of newly established lines of research, a programmatic funding of Euro 257 070 is recommended.

#### **#85#**

On the whole, quite impressive. A powerful array of equipment in well renovated laboratories.

The unit has a great problem of space, which it does not correspond neither to the number of researchers nor to the needs of the instrumentation.

Most of the groups are making some basic research, which can be a great interest if their results will be finally applied to other fields, like analytical chemistry. Thus, the sol-gel and similar studies can be very useful reagents for immobilisation, which is very interesting in flow techniques since it could allow saving expensive reagents in enzymatic reactions and immunoassays.

In a similar way, the studies of calyx(n)arenes and similar crown compounds (included cyclodextrins) could be of great interest if they could be immobilised in filters and the used to preconcentrate some analytes or their derivatives, since it could allow to reach lower limit levels and increase the selectivity of the analytical methods. Similar remarks may be done with fullerenes.

To help in upgrading several pieces of equipment that were recognized as holding back the medium term research planning of the unit, a programmatic funding of Euro 252 396 is recommended.

#### **#88#**

There is certainly some good work being done, by people who are well trained, competent and capable of original thought. This group is too small to aim at national recognition: only four researchers came to present their current projects, always on the synthesis of organic compounds. Among these, several should not be given a high priority and, given the means used, they cannot lead to very interesting results. As an example, the synthesis of alkaloids of the gephyrotoxine type has been extensively studied. The strategy used, which starts from a natural product, seems too long to be effective. On the other hand, the

starting product might be used to prepare new compounds of therapeutical potential. The same can be said about the synthesis of derivatives of tomosifen or the metal complexes. Only the topic on electron transfer appears to be truly original.

As individuals, therefore, they deserve encouragement, but, as a group, it is very difficult to see a successful future for them within the existing structure. The most effective suggestion, therefore, would be that they should be encouraged to integrate their existing group with a more flourishing one on the same campus.

### **#100#**

Unit 100 is a very large group (65 Ph.D. staff) with a broad cross section of interests and expertise in chemistry and chemical engineering. It is a large, competent and enthusiastic group of researchers. It is organized in six groups: (i) Bioinorganic, (ii) Organometallic and Catalysis, (iii) Statistical Mechanics and Thermochemistry, (iv) Molecular Photochemistry, (v) Coordination Chemistry and Electrochemistry and (vi) Chemistry and Electrochemistry of Natural Systems. This diverse unit correspondingly is characterized by a spectrum of age profiles and career achievements which range from young and inexperienced but very talented to relatively senior and experienced but undistinguished. Based on its standing in previous FCT evaluations, the group as a whole has apparently received relatively good funding in the past, however the committee was struck by the age of much of the equipment in use and the seeming inability to upgrade it. This is certainly one of the best structured and best organized units visited by the panel. The scientific production is strong and channelled to international journals.

Group I: The strengths of Group I are based almost entirely on the success of Dr. Fraústo da Silva's four books with R.J.P. Williams (Oxford), which are a major contribution to international scholarship. The research output of the group is quite adequate but would not be very exciting if that were all there was. Thus the future is not completely clear for Group I after the leader retires.

Group II: The expertise of the members of this group spans a wide range of areas, however the interactions within the group are such that they form a well integrated, interactive whole. They have a good deal of spectroscopic analytical services at their disposal including NMR, Mass Spectrometry and x-ray facilities. Their work on the preparation of catalysts follows well established principles but they also have an original outlook on the subject. The work on thermochemistry is also very good and addresses interesting problems in the energetics of organometallic species. On the whole the

scientific production is good. With the opportunity of moving into new well serviced space their interactions and productivity should increase even further.

Group III: From the Statistical Mechanics and Experimental Thermodynamics Group, the committee was struck by the dynamism and innovation of the work on molecular modelling of fluids and interfaces and the physical chemistry of surfaces and the synergy that existed between the principal participants. These young researchers have developed a cooperation which has quite clearly led to a situation where the sum of the parts is definitely greater than the whole and these individuals should be encouraged and supported. A number of other investigative avenues were pursued, in some cases involving rather dated experimental techniques for production of data with dubious application.

Group IV: One striking factor was the entirely inadequate space allotment to the Molecular Photochemistry Group which arguably is demonstrably the strongest group within the unit. This group has produced a significant number of high quality publications on chemical systems of imaginative design. The experiments have been well conceived and executed and one is left with the impression that the maximum information has been wrung from the equipment at hand.

Group V: This is a tremendously active group with a high standard in all areas. Many excellent publications have been produced in first class journals and a very strong culture of international cooperation exists (for example with Professor Kukushkin of St. Petersburg). However the group has less than six square meters per researcher and this should be remedied.

Group VI: The work being done by this group is adequate but unexciting and they appear to be the weakest in the unit. The results presented for this evaluation exercise are barely distinguishable from those presented at the 1999 evaluation.

Given the mix of quality of the individual groups within the unit, the overall rating recommended recognizes that some of the groups are excellent while others are average and should be understood as an encouragement to the search for excellence across the board.

This is a vast unit with good research facilities but several pieces of equipment needed upgrade and better technical support for their full utilization. A programmatic funding of Euro 607 620 and the unit should decide on its internal priorities in order to better fulfil the plans for the next few years.

**#248#**

This unit has carved out a very useful niche for itself: equipment and resources seem OK for projects being undertaken, but they would like (i) replacements for 3 PhD researchers who left recently to take up more permanent jobs, (ii) more chromatographic equipment, (iii) a mass spectrometry-liquid chromatography facility, and (iv) a molecular luminescence laboratory. The researchers are reasonably active and well organised and have good projects that do not seem to overlap much with others; their strength is in environmental analytical (not really inorganic, though they are interested in heavy metals and speciation). The most active publisher is Teresa Vasconcelos, on toxicity of chemicals. Projects include the study of the “bioavailable” fraction of the Pb present in digested red wines which is much lower than that present in the digested white wines; new threshold limits for Pb in wines; the  $^{87}\text{Sr}/^{86}\text{Sr}$  ratios can be a finger printer of the regional origin of wines” “Identification and quantification of ligands released by the roots of the wet-land plant *Cyperus eragrotis lam*” and Environmental chemometrics - Characterization of humic substances from soil, composted wastes, coastal seawater and river water and of their role in biogeochemical cycles.

Partners for collaboration have been identified (both in Portugal and Spain). Future projects include the development and optimisation of chemiluminescent sensors for screening of environmental pollutants, and, with a systems engineering group in Porto, fibre optic oxygen sensors based on newly synthesized platinum-group metal complexes with polypyridine. They should have more contacts with the institutions and companies working in this field.

The status of Basto has been resolved and is now satisfactory – she has been relocated in another group and is now productive. However the researchers are dissatisfied with interface to industry – they really need a person to “manage” and develop this aspect.

**#272# (Faro)**

It was not possible to make a preliminary assessment of this unit, because no information about it was provided until the moment of the site visit. At that time no explanation of the lack of material was offered, so no judgement can be made about whether this lack was in any way justifiable.

Despite the name of the unit, almost no biological chemistry is being done there; nor has any been done in the period covered by the list of publications, which include no references to journals normally read by biochemists. (Unit 411, also in Faro, is more biological than

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Unit 272.) The new director of the unit recognized that the name was inappropriate and needed to be changed, though he appeared not to accept this to be a priority. This is bound to have an adverse effect on the perception of a unit if its name bears no relation to the work being done. Even in the list of Objectives for 1999-2002 there was no mention of any biological chemistry, so a change of name would have been appropriate four years ago, if not long before.

The research publications for the period 1999-2002 represent an output of three to four papers in refereed journals per researcher. No SCI analysis could be made available for this unit, and the unit's own assessment of what constitutes a refereed journal appears optimistic (for example, is *Manuel de Zootechnie comparée Nord-Sud* a refereed journal), but even when the unit's estimate of 46 papers is corrected to a more realistic 36 it remains a respectable total for a small unit, and includes publications in some excellent journals, such as *J. Amer. Chem. Soc.* and *J. Phys. Chem.*

A difficulty for assessing the unit is that it appears to be on the threshold of a complete reorganization, not only with a new coordinator (Dr Eric Derouane, who joined it only in February 2003), but with the intention of developing new "horizontal research themes", with new collaborations, new industrial contacts, and new state-of-the-art equipment. All this is intended to take place in Year 1, with Year 2 expected to produce excellence in at least two research themes. However, this sequence appears to be unrealistic: acquisition of new equipment appears more likely to follow than to precede the achievement of excellence. Year 3 is intended to result in increased productivity by at least a factor of 2, with substantial additional funding generated through industrial collaboration. This last point also appears optimistic: discussions with other units suggests that it is far from easy to obtain substantial funding in the short term from industrial collaboration.

Nonetheless, it will be interesting to follow the future development of this Unit. If the objectives set out in the work plan are achieved it will constitute the first example in Portugal of a strong partnership between academic and private laboratories. Given Dr Derouane's experience in this domain it is realistic to hope it may be achieved. Success would mean creation of a joint venture with a large potential market.

### **#301#**

The Unit leader made a short presentation introducing their overall history and organization, following which each of the group leaders gave presentations of the statistics and activities of their individual groups. It came to light that these groups represented some of those that

were not invited to join Unit 612 when it was formed. With one exception these presentations were made difficult for the committee by the rather limited English language abilities of the speakers representing the groups. These presentations were followed by a laboratory tour in which the committee members divided themselves into two teams to visit the various groups. Mme. Camões gave an enthusiastic tour of the analytical facilities available to her to carry out her investigations. This work appeared to have a significant environmental interest and she was apparently well regarded within her discipline as indicated by her position as chair of an international committee. In the laboratory of kinetics of solution phase reactions, while the work appeared to be very carefully done and the data of high quality, a sense of chemical insight did not emanate from the presentations. Overall, little contact with the world outside academic research was detected and this is a sad remark as the labs available to the unit are rather nice. The scientific motivation of the pH and of the electroanalytical and environmental chemistry group was not clear. A group above the average is that on Molecular Simulation.

The group does not give a very dynamic impression. The scientific interest of the quaternization reactions is not clear. Few young researchers appear to be involved in new projects. With good laboratories, one would expect a much larger connection with the outside. The unit should consider the possibility of a deep reorganization, its members preferably joining some other more dynamic group or groups.

### **#313#**

The site visit created an extremely negative impression, leading to the conclusion that the unit is of a much lower standard than the written materials suggested. This was easily the most disappointing of all the Units visited. It was held two days later than originally scheduled, as some members were unable to be present at the original time. The evaluation panel was forced to make a second visit to Coimbra at considerable inconvenience, but at the start of the site visit it became clear that no preparations whatsoever had been made for it. There was no introductory presentation, the room in which it would have been held was locked, and the coordinator of the visit had no key. At no time did the panel have the opportunity of meeting the members of the unit as a whole. There were no posters collected together in a common place, and most of the laboratories had no posters on display. As far as one could discern no plans had been made for members of the panel to visit particular groups of relevance to them, with the result that these visits proceeded in a haphazard and unplanned way. In one lab we were told: "well, it is 5h30 on Friday afternoon, all the students have gone home – what do you expect?"

There is a group led by Dr Vaz that is concerned with biological chemistry, but no opportunity to visit his labs or discuss his work was offered.

Dr. Paliteiro presented his work in electrochemistry at great length but left no clear idea of what he was trying to do, or why. His explanation appeared a bit confused. He appeared to be trying to understand the reduction of molecular oxygen on metal electrodes entirely on the basis of electrochemical measurements, without using any data on the surface structures of the metals concerned. On being asked if he had any reprints that would allow a better understanding of his work he replied in terms that suggested that any lack of understanding was likely to be due to incompetence on the part of the panel members. However, it is not easy to ascertain which side is to blame for this difficulty in communication.

The performance of the unit as measured by the statistics appears to be high, so it is important to point out that the good results are due largely to a single group (Dr Varandas, theoretical chemistry) and that they give a misleading impression of the unit as a whole, which can be characterized at best as fair. The Photochemistry and Molecular Spectroscopy (PMS) Group as well as the Theoretical and Computational Chemistry Group were found to be particularly strong. In the case of the PMS group the equipment available was very good, at some cases at the forefront, and the problems investigated were novel. The experiments to probe the energetics of transient reaction intermediates were particularly interesting as were those on matrix isolation spectroscopy. The Theoretical Chemistry group (Varandas) was clearly tackling problems at the leading edge of the discipline. In the case of both groups the scientific production is substantial and the work is published in very high calibre journals. The investigators of these two groups are truly clearly world class.

In some groups, younger researchers should be given a more relevant role in the scientific leadership and in defining goals worth pursuing in the future. Connections with industry, in Portugal or beyond, must be encouraged so that the relevant problems are tackled.

The panel that made the previous evaluation of the unit in 1999 expressed a strong desire to see the problems of the poor relations between it and other researchers in Coimbra resolved as quickly as possible. It is thus very disappointing to see that more than three years later some members of the unit are now engaged in litigation about the same problems that were evident in 1999. It is hard to escape the conclusion that investment by the FCT in this unit is likely to be in part wasted, and that it should be minimal until the University takes the proper steps to end the dispute.

**#612#**

The CQB Unit is a newly formed research unit made up of groups formerly housed in a number of other research units. The new unit has 37 members distributed in 18 separate research groups with a wide range of interests across several areas of Chemistry. In this respect the unit bears a strong resemblance to the graduate research faculty of a large Chemistry department. In some cases there are intersections of interest between groups but to a large extent they exist completely independently of each other. The unit is housed in a most impressive new facility which was opened in 2001 and which is well serviced for modern research in Chemistry. Following a general introduction by the Unit Director, the committee members attended a poster presentation by each of the groups within the Unit. Because of the large size of the Unit the posters visited by the committee were divided among the members. This was followed by a tour of the laboratories themselves. Overall the groups within the unit appear to have been well chosen in terms of representing areas of strength within their individual disciplines. Given the very large number of groups within the unit, detailed comments on each one were not possible. Of particular note are the groups in Inorganic and Computational Chemistry, Interfacial Electrochemistry, Carbohydrate Chemistry and Molecular Energetics where both the quality of the work carried out and the level of scientific production were very high. The Carbohydrate Chemistry group has results that are totally original and may lead to many applications in domains of the interface between chemistry and biology. It should be given priority finance. A number of the groups within the unit have a distinct biochemical focus or have a biochemical component. None of these are the most highly ranked groups within the unit, however Molecular Biophysics and Biocatalysis groups were deemed to be above average within the unit. Similarly, the Interfacial Electrochemistry Group was found to be above average. Nonetheless, nearly all of the biochemical groups have a good level of production, and the Enzymology (Ponces) and Oxidants and Antioxidants (Marinho) groups deserve particular mention for the original and modern nature of their work in well established domains. The weakest members of the unit were perceived to be the Biochemistry of Selenium, Mass Spectrometry, Solvent Extraction and Interfacial and Supramolecular Chemistry groups.

There appear to exist too many groups in Portugal interested in vanadium compounds. A sole group putting together all the resources would suffice. The goals of the work on Free Radical Biochemistry, Organic Compounds and solvent Extraction for Metal Recover need a careful rethinking.



The potential of the whole unit is very interesting and the cohesion appears to be high. The researchers should engage into thinking their future and chose to reinforce the topics of highest breath and perhaps leaving other topics. Given the very heterogeneous nature of this unit it was somewhat difficult to arrive at a final overall rating. The final value takes all factors into account and is intended as an incentive for the future.

This is a newly formed unit where a strong internal coordination needs a programmatic funding that is recommended at the level of Euro 403 522 for its better strategic guidance.

### **#619#**

This is a newly formed unit within the Chemistry Department of the University of Évora. The Chemistry Department has grown rapidly in recent years as has the number of faculty holding Ph.D. degrees. This new unit is now composed of more than 15 PhD permanents. The unit has proposed projects in analytical, organic, inorganic, physical and theoretical chemistry as well as biotechnology. Both fundamental and applied investigations are foreseen. A number of projects have already been funded under other programs from both the FCT and other agencies. The Committee did not have the opportunity to speak with all investigators in the proposed unit, however during a tour of the laboratories a number of the projects in progress were explained. The most developed of these was the research of the unit leader, Professor Carrott, who with M.M.L. Ribeiro Carrott, has a program of investigation of absorption of a variety of materials on activated carbon fibres derived from a number of sources including acrylic textile fibres and cork. Other related studies are carried out on zeolites. The laboratory is relatively well equipped for these studies and includes a powder x-ray diffractometer, recently purchased with external funding. This is a very impressive resource to be found in such a fledgling unit. Another effort, which appears to have gotten off to a healthy start, is in the area of organic synthesis using novel reagents. Similarly there seems to be good expertise in the analysis of thermodynamics of mixtures of unconventional liquids. There is considerable potential here to gain understanding of intermolecular forces in unusual environments.

The physical plant available to the unit has a number of serious limitations. Firstly, they must share their research laboratories with upper year undergraduate chemistry laboratories. Secondly, the conversion of the former barracks stable to laboratory space is considerably less than optimal. In particular, a proper venting of fume hoods must be undertaken for simple health and safety reasons.

Three main topics are developed in the organic chemistry group:

- Organometallics: New organometallics have been synthesized for their non-linear optical properties. The research program involves rational modifications in order to improve the properties of the synthesized compounds. However, it seems that no important new results have recently been obtained. Furthermore the lack of facilities (mainly NMR) seriously obliterates the possibility of success in this project.
- Asymmetric catalysis: An enthusiastic young researcher who studies the preparation of new ligands for asymmetric catalysis.
- Natural product studies: This is a traditional area of research in this University. Several families of compounds have been isolated from various plants. The method to find new active compounds implies successive evaluations of extracts to focalise on the potentially active compounds.

The overall impression is mixed. There is a general lack of enthusiasm of researchers and also of ambitious projects.

While recognizing that this proposed unit has made modest contributions, on the whole, to research to date, there was considerable sympathy to the situation in which the members find themselves. In addition, the determination and enthusiasm of many of the unit members to begin a research enterprise was impressive. In view of this, the Committee was of the opinion that the Unit should be given the opportunity to make a start in this direction and as a result an evaluation of "2" is recommended in order that some FCT funding flow to them to subsidize some of their more immediate research needs.

#### **#411#**

The CMQA proposed research unit has been created to focus on problems in Environmental Chemistry. Even though the members of the unit have a wide range of backgrounds in various disciplines a mission has been established to direct the efforts of their various areas of expertise on problems of the environment. The unit is sub-divided into five groups.

The first of these is in Photodegradation of Pollutants. This group has had a very modest publication history but they also run an analytical service for water and organic matter for various agencies in the Algarve region which necessarily occupies a considerable fraction of their time. Probably they are more engaged with chemical analysis than in analytical chemistry, since most of these studies are merely a recompilation of data values which may allow to evaluation the situation of their environment. This could be interesting in an initial

step, but in the future they should do more analytical chemistry developing new methodologies better adapted to their needs.

The second group is in the area of Marine Environmental Chemistry, in particular in the study of the eutrophication of local waters. This group was perceived to be doing some useful analytical chemistry work which benefits the region.

The Biochemistry group has only recently come together and are still seeking a common goal but are headed in the direction of examination of the effects of metals as well as other xenobiotics on biological systems. There has been no substantive contribution of this group to date however.

The fourth group is in the area of theoretical chemistry. This might seem to be the most difficult area to fit into an environmental research perspective but in fact the focus of the theoretical work to date has been on potential energy surfaces for reactions of atmospheric importance. There are substantial computer resources available for this work in the form of a 8 CPU Beowulf cluster and a DEC system. The background of the group (and unit) leader is excellent for such work.

The final group is directed toward the study of metals in natural systems and includes investigation of the mechanism of toxicity vanadium and its derivatives.

The general impression is that some of these works are interesting examples of application but could not constitute strong fields of research. The exceptions may be the study of proteins involved in cork oak diseases and perhaps the study of the mechanism of the toxicity of vanadium derivatives. However this last area of research is also studied in other laboratories in Portugal. It would be interesting to understand the origins of such an interest for vanadium derivatives as none of the visited laboratories had real collaboration with industrial companies in this field despite the obvious interest of this research.

Overall there was not a strong impression that the research efforts of the unit were, in fact, well unified but the Committee felt that there was the potential for a reasonable research effort to grow if the unit were given the opportunity to develop, albeit under constrained circumstances. Accordingly, a rating of 2 is recommended in order the some funding flow to the unit to support its research activities and to provide it an entry into the FCT funding system.

**#536#**

The Centre for Molecular Science and Materials (CCMM) is divided into two sub-units one of which is a unit of Chemistry and the other a unit of the Chemistry and Physics of Solids. The evaluation Committee was asked to make a recommendation only on the former unit, however a last minute presentation by Professor Elias, from the latter sub-unit, on glass forming materials was added to the in camera presentations. The Chemistry sub-unit is further divided into two groups: Thermophysics and Structural Chemistry and Biochemistry. The unifying theme for this sub-unit appeared to be the very applied nature of their work and in a North American university they might be found more naturally in a Chemical Engineering department rather than a Chemistry Department.

The Thermophysics group is concerned primarily with high temperature materials, in particular their transport properties and thermal conductivity. In addition some experiments are in progress on materials characterization for refrigerants, intermolecular interactions in liquids and solutions and properties of materials under microgravity. The laboratory was extraordinarily well equipped with heavy equipment and the co-workers of Professor de Castro were very knowledgeable and enthusiastic about their research. Apparently he now spends a large amount of his time in a government administrative appointments although he appears to continue to be well versed in the activities of the group that he directs. The scientific production was relatively modest for a group of this size however.

The second group is further divided into three research themes: Physical Organic Chemistry, Analytical Chemistry and Biochemistry. The first theme, headed by Professor Pereira concerns calixerenes and their characterization and application to binding of metal ions. The second theme of a relatively new appointee, Professor Nogueira, is just getting underway. His laboratory that has received equipment and analytical work is in the initial phases. The final theme is in applied biochemistry, directed by Professor Barata and is directed to structural and functional relationships of proteins in unusual environments as well as possible economic applications of these. He might consider the relocation of his group to another research unit. The publication output is again rather modest in part due to the relatively junior status of two of the team leaders. In each case however well serviced and well equipped laboratories are available to the investigators. The work in three of the cases appeared to be of high quality and the space and equipment resources to carry out the research were very good. The two younger members had a limited number of co-workers but it would be anticipated that this would change with time as they become better established. Globally, there appears to be a lack of PhD students what may be associated with a low attractivity of the group.

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No attempt was made to assess the research of the glass forming materials group of Prof. Anselmo Elias who might fit better elsewhere.

A programmatic funding of Euro 51 414 is proposed, suggesting that a improved technical support will improve the unit results.

### **#616# ( Vila-Real)**

This is a new unit putting together young and enthusiastic researchers with interesting projects. They suffer from he lack of heavy analytical equipment and on line library. The scientific production is good. There are three research groups:

- organic chemistry. Very young and dynamic, they work on the synthesis of photochromic molecules, cyanines dyes with photodynamic properties for cancer treatment and on chromones. All his work is done incollaboration with other groups that take on the responsibility for the evaluation of the physical and biological properties.
- Solid state chemistry. Preparation organic/inorganic mixed materials and study of their physical properties. So-gel techniques and ceramics.
- Analytical chemistry. Study of the oxidative degradation of pollutants. There is also an interesting experience on the production of tartaric acid as a by product of the wine industry.

The major difficulty for evaluating this unit comes from the fact that most work is done in collaboration with other groups and it is not easy to assess what is actually done in Vila Real and to how far does the originality of the group go. They should be given a chance to prove themselves.

An energetic group of young researchers working in an environment very difficult for performing research. The themes developed were interesting and each had an applied focus. The solid-state chemistry group was particularly strong in terms of publications and activity. There was a perceived effort by many members of the unit to overcome the difficulties of performing research in Vila Real by going elsewhere for key instrumental needs. The desire to develop key instrument resources at Vial Real was perhaps premature since the demand for example for NMR in house could not occupy and instrument full time. However if the productivity of the solid-state chemistry group were to continue a case could eventually be made for a modern in house powder x-ray facility.

The final rating proposed should be seen as tentative and as an incentive that waits confirmation in the future.

A programmatic funding of Euro 49 077 is proposed as seed money to the improvement of some of the recognized limitations in the research equipment available to the unit. The panel recognizes a high potential in this research unit and suggests that it may negotiate with the University the co-funding of some of its financial requirements to make it into one of the flagships of research in Vila Real in the next round of evaluation.

#### **#674# (Funchal)**

This is a new unit made from the teamwork of 7 PhDs of the Chemistry Department of Madeira University. Its creation is too recent (2002) to have given enough time to the group to obtain a scientific production, which could be the object of an evaluation.

However the enthusiasm of the group, the good laboratories and the quality of the projects constitute a promising starting point for the future. The major problems due to isolation, far from the main centres of research in Portugal, to the small size of the population in Madeira, and to the low level of financial investment in chemical research in Madeira. Although the researchers can in principle have samples analysed by NMR, mass spectroscopy, etc., at centres on the continent, they report that in practice this can take as long as six months because their samples are given very low priority. This is an extreme case of a general problem for smaller units located in remote parts of Portugal. It would hardly be feasible to solve it by providing a complete range of modern equipment in each small centre, but one could think, perhaps, of finding a solution in terms of a service unit with a primary responsibility of satisfying the needs of researchers in remote centres.

Two major lines are developed in the group: Natural Products and Materials. The coordinator of the group, Dr Marques, is engaged in applied research related to the Madeira wine industry, and has established good relations with the producers, who are interested in the results that he is obtaining. Aromatic characterisation, impact of ageing processes and biological pest control constitute the main research topics of the group. Some minor studies are devoted to isolation and characterisation of compounds from plants.

In the Materials research line, the synthesis and study of new organometallic dendrimers is the most advanced project. Some interesting applications to optoelectronic and environmental studies are scheduled. The second project dealing with bone tissue engineering needs a little more time to be really evaluated; it is being developed in collaboration with Madeira hospital and could furnish original results in a near future. The

work by Dr Tomás has not yet led to any publications, and it is therefore premature to make a definitive evaluation, but it appears to be well conceived and relevant to medical problems.

The interest of the research is confirmed by the approval of 6 projects since 2000, in equal parts in the two domains of activity. One of the projects is financed through the E.C. (INTERREG).

The main problem of this group is the absence of funds to equip its laboratories and to become attractive to new students. It is necessary to keep equilibrium between applied and innovative chemistry. The limited number of researchers obliged the group to limit its areas of research. It is absolutely necessary to give a chance to this young enthusiastic team and to study the progress in a next evaluation, to see how far they could go in finding and developing interesting and solid research ideas of their own with the depth and breadth expected of a university research group.

#### **#686# (Braga)**

This unit is composed with 38 PhD permanents. The main area of research is organic chemistry synthesis with three well defined and complementary topics: Biological Chemistry, Chemistry of Heterocyclic Compounds and Peptide Chemistry. A fourth area is Physical and Analytical Chemistry.

On Heterocyclic Chemistry, the main research topics are the synthesis of 3 to 7 membered heterocycles containing polycyclic structures with nitrogen, sulphur and oxygen atoms. It's a very classical chemistry leading to polyfunctionalized compounds, which could find applications in various domains. However, one does not get the impression that it is the major preoccupation of the researchers of this group. Some of the results presented, especially those involving the preparation of pyrazoles and pyrazolopyrimidines via the addition of an amine to a reactive cyano derivative, could be easily applied to the creation of original chimiotheques, which could be of relevant interest for foreign industrial companies. The project on the synthesis of electrophilic azirines is similar to another developed in Coimbra. The researcher involved in this project would have to give a more original orientation to his work.

On Peptide Chemistry, some very original and interesting results are encountered in this group. The synthesis of new non-proteogenic aminoacids and the results obtained with the Ugi reaction are very promising. In a near future, it would be very useful to study an asymmetric version of the methodologies developed in this group.

The group in Biological Chemistry follows an interesting line of work. The biological degradation of azo dyes is studied in collaboration with three other centres and with contacts with local industries. The synthesis of glycoconjugates of metal complexes for medical applications realized in collaboration with the NMR Laboratory of Coimbra and Braga hospital is of great interest and can be considered as a major subject of research in this group. This methodology can be applied to many biological targets via the modification of the sugar part. The third project, on therapeutic biomolecule purification, seems to be interesting.

Physical Chemistry and Analytical Chemistry: The group of physical and analytical chemistry is currently working mainly in physical chemistry with some very interesting subjects, like the integration of the semiconductors with sol-gel techniques. They are also involved in some electrochemical topics of high interest, such as electrosynthesis and electrodegradation. With the use of microelectrodes, they are able to obtain good results in the study of some pollutants.

In conclusion unit 686 gave a very good impression for the originality of its results as well as the dynamism of the researchers: Many young chemists are involved in promising projects and seem to be free to develop their own research. However this unit suffers of a lack of specialized apparatus such as NMR and budget cut-backs of the University.

The final rating proposed should be seen as tentative and as a strong incentive for the future performance of the group, especially of its younger members. A programmatic funding of Euro 236 816 is recommended to support the autonomy required to make some of the younger and more promising researchers in the unit into internationally recognized first rank scientists.

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