



INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL  
TRAINING AT THE UNIVERSITY OF HELSINKI 2005–2010

# RC-Specific Evaluation of MEDCHEMBIO – Medicinal Chemistry and Biochemistry Research Group

Seppo Saari & Antti Moilanen (Eds.)



Evaluation Panel: Natural Sciences



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University of Helsinki  
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<b>Title:</b> International Evaluation of Research and Doctoral Training at the University of Helsinki 2005–2010 : RC-Specific Evaluation of MEDCHEMBIO – Medicinal Chemistry and Biochemistry Research Group	<b>Type of publication:</b> Evaluations
<b>Summary:</b> Researcher Community (RC) was a new concept of the participating unit in the evaluation. Participation in the evaluation was voluntary and the RCs had to choose one of the five characteristic categories to participate. Evaluation of the Researcher Community was based on the answers to the evaluation questions. In addition a list of publications and other activities were provided by the TUHAT system. The CWTS/Leiden University conducted analyses for 80 RCs and the Helsinki University Library for 66 RCs. Panellists, 49 and two special experts in five panels evaluated all the evaluation material as a whole and discussed the feedback for RC-specific reports in the panel meetings in Helsinki. The main part of this report is consisted of the feedback which is published as such in the report. Chapters in the report: 1. Background for the evaluation 2. Evaluation feedback for the Researcher Community 3. List of publications 4. List of activities 5. Bibliometric analyses The level of the RCs' success can be concluded from the written feedback together with the numeric evaluation of four evaluation questions and the category fitness. More conclusions of the success can be drawn based on the University-level report.	
<b>RC-specific information:</b>	
<b>Main scientific field of research:</b> Natural Sciences	<b>RC-specific keywords:</b> medicinal chemistry, drug discovery, drug metabolism, molecular modelling, organic synthesis, pharmacy
<b>Participation category:</b> 4. Research of the participating community represents an innovative opening	
<b>RC's responsible person:</b> Yli-Kauhaluoma, Jari	
<b>Keywords:</b> Research Evaluation, Meta-evaluation, Doctoral Training, Bibliometric Analyses, Researcher Community	

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## Foreword

The evaluation of research and doctoral training is being carried out in the years 2010–2012 and will end in 2012. The steering group appointed by the Rector in January 2010 set the conditions for participating in the evaluation and prepared the Terms of Reference to present the evaluation procedure and criteria. The publications and other scientific activities included in the evaluation covered the years 2005–2010.

The participating unit in the evaluation was defined as a Researcher Community (RC). To obtain a critical mass with university-level impact, the number of members was set to range from 20 to 120. The RCs were required to contain researchers in all stages of their research career, from doctoral students to principal investigators (PIs). All in all, 136 Researcher Communities participated in this voluntary evaluation, 5857 persons in total, of whom 1131 were principal investigators. PIs were allowed to participate in two communities in certain cases, and 72 of them used this opportunity and participated in two RCs.

This evaluation enabled researchers to define RCs from the “bottom up” and across disciplines. The aim of the evaluation was not to assess individual performance but a community with shared aims and researcher-training activities. The RCs were able to choose among five different categories that characterised the status and main aims of their research. The steering group considered the process of applying to participate in the evaluation to be important, which led to the establishment of these categories. In addition, providing a service for the RCs to enable them to benchmark their research at the global level was a main goal of the evaluation.

The data for the evaluation consisted of the RCs’ answers to evaluation questions on supplied e-forms and a compilation extracted from the TUHAT – Research Information System (RIS) on 12 April 2011. The compilation covered scientific and other publications as well as certain areas of scientific activities. During the process, the RCs were asked to check the list of publications and other scientific activities and make corrections if needed. These TUHAT compilations are public and available on the evaluation project sites of each RC in the TUHAT-RIS.

In addition to the e-form and TUHAT compilation, University of Leiden (CWTS) carried out bibliometric analyses from the articles included in the Web of Science (WoS). This was done on University and RC levels. In cases where the publication forums of the RC were clearly not represented by the WoS data, the Library of the University of Helsinki conducted a separate analysis of the publications. This was done for 66 RCs representing the humanities and social sciences.

The evaluation office also carried out an enquiry targeted to the supervisors and PhD candidates about the organisation of doctoral studies at the University of Helsinki. This and other documents describing the University and the Finnish higher education system were provided to the panellists.

The panel feedback for each RC is unique and presented as an entity. The first collective evaluation reports available for the whole panel were prepared in July–August 2011. The reports were accessible to all panel members via the electronic evaluation platform in August. Scoring from 1 to 5 was used to complement written feedback in association with evaluation questions 1–4 (scientific focus and quality, doctoral training, societal impact, cooperation) and in addition to the category evaluating the fitness for participation in the evaluation. Panellists used the international level as a point of comparison in the evaluation. Scoring was not expected to go along with a preset deviation.

Each of the draft reports were discussed and dealt with by the panel in meetings in Helsinki (from 11 September to 13 September or from 18 September to 20 September 2011). In these meetings the panels also examined the deviations among the scores and finalised the draft reports together.

The current RC-specific report deals shortly with the background of the evaluation and the terms of participation. The main evaluation feedback is provided in the evaluation report, organised according to the evaluation questions. The original material provided by the RCs for the panellists has been attached to these documents.

On behalf of the evaluation steering group and office, I sincerely wish to thank you warmly for your participation in this evaluation. The effort you made in submitting the data to TUHAT-RIS is gratefully acknowledged by the University. We wish that you find this panel feedback useful in many ways. The bibliometric profiles may open a new view on your publication forums and provide a perspective for discussion on your choice of forums. We especially hope that this evaluation report will help you in setting the future goals of your research.

Johanna Björkroth  
Vice-Rector  
Chair of the Steering Group of the Evaluation

### **Steering Group of the evaluation**

Steering group, nominated by the Rector of the University, was responsible for the planning of the evaluation and its implementation having altogether 22 meetings between February 2010 and March 2012.

### **Chair**

Vice-Rector, professor **Johanna Björkroth**

### **Vice-Chair**

Professor **Marja Airaksinen**

Chief Information Specialist, Dr **Maria Forsman**

Professor **Arto Mustajoki**

University Lecturer, Dr **Kirsi Pyhälä**

Director of Strategic Planning and Development, Dr **Ossi Tuomi**

Doctoral candidate, MSocSc **Jussi Vauhkonen**



# Panel members

## **CHAIR**

### **Professor Jan-Otto Carlsson**

Materials science in chemistry and physics, nanotechnology, inorganic chemistry  
Uppsala University, Sweden

## **VICE-CHAIR**

### **Professor Jan van Leeuwen**

Computer science, information technology  
University of Utrecht, the Netherlands

### **Professor Caitlin Buck**

Probability and statistics, archeology, palaeoenvironmental science  
University of Sheffield, Great Britain

### **Professor David Colton**

Mathematics, inverse problems of acoustic and electromagnetic scattering  
University of Delaware, USA

### **Professor Jean-Pierre Eckmann**

Mathematics, dynamical systems, mathematical physics  
University of Geneva, Switzerland

### **Professor Ritske Huismans**

Geosciences, geodynamics  
University of Bergen, Norway

### **Professor Jukka Jurvelin**

Medical physics and engineering  
University of Eastern Finland

### **Professor Lea Kauppi**

Environmental sciences, water research  
The Finnish Environment Institute, Finland

### **Professor Riitta Keiski**

Chemical engineering, heterogeneous catalysis, environmental technology, mass and heat transfer processes  
University of Oulu, Finland

### **Professor Mats Larsson**

Experimental molecular physics, chemical dynamics, molecular spectroscopy, astrobiology  
Stockholm University, Sweden

### **Professor Holger Stark**

Medicinal, organic and pharmaceutical chemistry, pharmacology  
Johann Wolfgang Goethe Universität, Germany

The panel, independently, evaluated all the submitted material and was responsible for the feedback of the RC-specific reports. The panel members were asked to confirm whether they had any conflict of interests with the RCs. If this was the case, the panel members disqualified themselves in discussion and report writing.

Added expertise to the evaluation was contributed by the members from the other panels.

### **Experts from the Other Panels**

**Professor Barbara Koch**, from the Panel of Biological, Agricultural and Veterinary Sciences

**Professor Peter York**, from the Panel of Medicine, Biomedicine and Health Sciences

### **EVALUATION OFFICE**

**Dr Seppo Saari, Doc.**, Senior Adviser in Evaluation, was responsible for the entire evaluation, its planning and implementation and acted as an Editor-in-chief of the reports.

**Dr Eeva Sievi, Doc.**, Adviser, was responsible for the registration and evaluation material compilations for the panellists. She worked in the evaluation office from August 2010 to July 2011.

**MSocSc Paula Ranne**, Planning Officer, was responsible for organising the panel meetings and all the other practical issues like agreements and fees and editing a part the RC-specific reports. She worked in the evaluation office from March 2011 to January 2012.

**Mr Antti Moilanen**, Project Secretary, was responsible for editing the reports. He worked in the evaluation office from January 2012 to April 2012.

### **TUHAT OFFICE**

#### **Provision of the publication and other scientific activity data**

**Mrs Aija Kaltera**, Project Manager of TUHAT-RIS served the project ex officio providing the evaluation project with the updated information from TUHAT-RIS. The TUHAT office assisted in mapping the publications with CWTS/University of Leiden.

**MA Liisa Ekebon**, Assisting Officer, served in TUHAT-RIS updating the publications for the evaluation. She also assisted the UH/Library analyses.

**BA Liisa Jäppinen**, Assisting Officer, served in TUHAT-RIS updating the publications for the evaluation.

### **HELSINKI UNIVERSITY LIBRARY**

#### **Provision of the publication analyses**

**Dr Maria Forsman**, Chief Information Specialist in the Helsinki University Library, managed with her 10 colleagues the bibliometric analyses in humanities, social sciences and in other fields of sciences where CWTS analyses were not applicable.

## **Acronyms and abbreviations applied in the report**

### **External competitive funding**

AF - Academy of Finland  
TEKES - Finnish Funding Agency for Technology and Innovation  
EU - European Union  
ERC - European Research Council  
International and national foundations  
FP7/6 etc. /Framework Programmes/Funding of European Commission

### **Evaluation marks**

Outstanding (5)  
Excellent (4)  
Very Good (3)  
Good (2)  
Sufficient (1)

### **Abbreviations of Bibliometric Indicators**

P - Number of publications  
TCS - Total number of citations  
MCS - Number of citations per publication, excluding self-citations  
PNC - Percentage of uncited publications  
MNCS - Field-normalized number of citations per publication  
MNJS - Field-normalized average journal impact  
THCP10 - Field-normalized proportion highly cited publications (top 10%)  
INT\_COV - Internal coverage, the average amount of references covered by the WoS  
WoS - Thomson Reuters Web of Science Databases

### **Participation category**

Category 1. The research of the participating community represents the international cutting edge in its field.

Category 2. The research of the participating community is of high quality, but the community in its present composition has yet to achieve strong international recognition or a clear break-through.

Category 3. The research of the participating community is distinct from mainstream research, and the special features of the research tradition in the field must be considered in the evaluation.

Category 4. The research of the participating community represents an innovative opening.

Category 5. The research of the participating community has a highly significant societal impact.

### **Research focus areas of the University of Helsinki**

Focus area 1: The basic structure, materials and natural resources of the physical world

Focus area 2: The basic structure of life

Focus area 3: The changing environment - clean water

Focus area 4: The thinking and learning human being

Focus area 5: Welfare and safety

Focus area 6: Clinical research

Focus area 7: Precise reasoning

Focus area 8: Language and culture

Focus area 9: Social justice

Focus area 10: Globalisation and social change



# 1 Introduction to the Evaluation

## 1.1 RC-specific evaluation reports

The participants in the evaluation of research and doctoral training were Researcher Communities (hereafter referred to as the RC). The RC refers to the group of researchers who registered together in the evaluation of their research and doctoral training. Preconditions in forming RCs were stated in the Guidelines for the Participating Researcher Communities. The RCs defined themselves whether their compositions should be considered well-established or new.

It is essential to emphasise that the evaluation combines both meta-evaluation<sup>1</sup> and traditional research assessment exercise and its focus is both on the research outcomes and procedures associated with research and doctoral training. The approach to the evaluation is enhancement-led where self-evaluation constituted the main information. The answers to the evaluation questions formed together with the information of publications and other scientific activities an entity that was to be reviewed as a whole.

The present evaluation recognizes and justifies the diversity of research practices and publication traditions. Traditional Research Assessment Exercises do not necessarily value high quality research with low volumes or research distinct from mainstream research. It is challenging to expose the diversity of research to fair comparison. To understand the essence of different research practices and to do justice to their diversity was one of the main challenges of the present evaluation method. Understanding the divergent starting points of the RCs demanded sensitivity from the evaluators.

## 1.2 Aims and objectives in the evaluation

The aims of the evaluation are as follows:

- to improve the level of research and doctoral training at the University of Helsinki and to raise their international profile in accordance with the University's strategic policies. The improvement of doctoral training should be compared to the University's policy.<sup>2</sup>
- to enhance the research conducted at the University by taking into account the diversity, originality, multidisciplinary nature, success and field-specificity,
- to recognize the conditions and prerequisites under which excellent, original and high-impact research is carried out,
- to offer the academic community the opportunity to receive topical and versatile international peer feedback,
- to better recognize the University's research potential.
- to exploit the University's TUHAT research information system to enable transparency of publishing activities and in the production of reliable, comparable data.

## 1.3 Evaluation method

The evaluation can be considered as an enhancement-led evaluation. Instead of ranking, the main aim is to provide useful information for the enhancement of research and doctoral training of the participating RCs. The comparison should take into account each field of science and acknowledge their special character.

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<sup>1</sup> The panellists did not read research reports or abstracts but instead, they evaluated answers to the evaluation questions, tables and compilations of publications, other scientific activities, bibliometrics or comparable analyses.

<sup>2</sup> [Policies on doctoral degrees and other postgraduate degrees at the University of Helsinki.](#)

The comparison produced information about the present status and factors that have led to success. Also challenges in the operations and outcomes were recognized.

The evaluation approach has been designed to recognize better the significance and specific nature of researcher communities and research areas in the multidisciplinary top-level university. Furthermore, one of the aims of the evaluation is to bring to light those evaluation aspects that differ from the prevalent ones. Thus the views of various fields of research can be described and research arising from various starting points understood better. The doctoral training is integrated into the evaluation as a natural component related to research. Operational processes of doctoral training are being examined in the evaluation.

**Five stages of the evaluation method were:**

1. Registration – Stage 1
2. Self-evaluation – Stage 2
3. TUHAT<sup>3</sup> compilations on publications and other scientific activities<sup>4</sup>
4. External evaluation
5. Public reporting

## 1.4 Implementation of the external evaluation

### Five Evaluation Panels

Five evaluation panels consisted of independent, renowned and highly respected experts. The main domains of the panels are:

1. biological, agricultural and veterinary sciences
2. medicine, biomedicine and health sciences
3. natural sciences
4. humanities
5. social sciences

The University invited 10 renowned scientists to act as chairs or vice-chairs of the five panels based on the suggestions of faculties and independent institutes. Besides leading the work of the panel, an additional role of the chairs was to discuss with other panel chairs in order to adopt a broadly similar approach. The panel chairs and vice-chairs had a pre-meeting on 27 May 2011 in Amsterdam.

The panel compositions were nominated by the Rector of the University 27 April 2011. The participating RCs suggested the panel members. The total number of panel members was 50. The reason for a smaller number of panellists as compared to the previous evaluations was the character of the evaluation as a meta-evaluation. The panellists did not read research reports or abstracts but instead, they evaluated answers to the evaluation questions, tables and compilations of publications, other scientific activities, bibliometrics and comparable analyses.

The panel meetings were held in Helsinki:

- On 11–13 September 2011: (1) biological, agricultural and veterinary sciences, (2) medicine, biomedicine and health sciences and (3) natural sciences.
- On 18–20 September 2011: (4) humanities and (5) social sciences.

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<sup>3</sup> TUHAT (acronym) of Research Information System (RIS) of the University of Helsinki

<sup>4</sup> Supervision of thesis, prizes and awards, editorial work and peer reviews, participation in committees, boards and networks and public appearances.

## 1.5 Evaluation material

The main material in the evaluation was the RCs' self-evaluations that were qualitative in character and allowed the RCs to choose what was important to mention or emphasise and what was left unmentioned.

The present evaluation is exceptional at least in the Finnish context because it is based on both the evaluation documentation (self-evaluation questions, publications and other scientific activities) and the bibliometric reports. All documents were delivered to the panellists for examination.

Traditional bibliometrics can be reasonably done mainly in medicine, biosciences and natural sciences when using the Web of Science database, for example. Bibliometrics, provided by CWTS/The Centre for Science and Technology Studies, University of Leiden, cover only the publications that include WoS identification in the TUHAT-RIS.

Traditional bibliometrics are seldom relevant in humanities and social sciences because the international comparable databases do not store every type of high quality research publications, such as books and monographs and scientific journals in other languages than English. The Helsinki University Library has done analysis to the RCs, if their publications were not well represented in the Web of Science databases (RCs should have at least 50 publications and internal coverage of publications more than 40%) – it meant 58 RCs. The bibliometric material for the evaluation panels was available in June 2011. The RC-specific bibliometric reports are attached at the end of each report.

The panels were provided with the evaluation material and all other necessary background information, such as the basic information about the University of Helsinki and the Finnish higher education system.

### Evaluation material

1. Registration documents of the RCs for the background information
2. Self evaluation material – answers to the evaluation questions
3. Publications and other scientific activities based on the TUHAT RIS:
  - 3.1. statistics of publications
  - 3.2. list of publications
  - 3.3. statistics of other scientific activities
  - 3.4. list of other scientific activities
4. Bibliometrics and comparable analyses:
  - 4.1. Analyses of publications based on the verification of TUHAT-RIS publications with the Web of Science publications (CWTS/University of Leiden)
  - 4.2. Publication statistics analysed by the Helsinki University Library - mainly for humanities and social sciences
5. University level survey on doctoral training (August 2011)
6. University level analysis on publications 2005–2010 (August 2011) provided by CWTS/University of Leiden

### Background material

University of Helsinki

- [Basic information about the University of the Helsinki](#)
- [The structure of doctoral training at the University of Helsinki](#)
- Previous evaluations of research at the University of Helsinki – links to the reports: [1998](#) and [2005](#)

The Finnish Universities/Research Institutes

- [Finnish University system](#)
- [Evaluation of the Finnish National Innovation System](#)
- [The State and Quality of Scientific Research in Finland. Publication of the Academy of Finland 9/09.](#)

The evaluation panels were provided also with other relevant material on request before the meetings in Helsinki.

## 1.6 Evaluation questions and material

The participating RCs answered the following evaluation questions which are presented according to the evaluation form. In addition, TUHAT RIS was used to provide the **additional material** as explained. For giving the feedback to the RCs, the panellists received the evaluation feedback form constructed in line with the evaluation questions:

### 1. Focus and quality of the RC's research

- Description of
  - the RC's research focus.
  - the quality of the RC's research (incl. key research questions and results)
  - the scientific significance of the RC's research in the research field(s)
- Identification of the ways to strengthen the focus and improve the quality of the RC's research

The additional material: TUHAT compilation of the RC's publications, analysis of the RC's publications data (provided by University of Leiden and the Helsinki University Library)

A written feedback from the aspects of: scientific quality, scientific significance, societal impact, innovativeness

- Strengths
- Areas of development
- Other remarks
- Recommendations

Numeric evaluation: OUTSTANDING (5), EXCELLENT (4), VERY GOOD (3), GOOD (2), SUFFICIENT (1)

### 2. Practises and quality of doctoral training

- Organising of the doctoral training in the RC. Description of the RC's principles for:
  - recruitment and selection of doctoral candidates
  - supervision of doctoral candidates
  - collaboration with faculties, departments/institutes, and potential graduate schools/doctoral programmes
  - good practises and quality assurance in doctoral training
  - assuring of good career perspectives for the doctoral candidates/fresh doctorates
- Identification of the RC's strengths and challenges related to the practises and quality of doctoral training, and the actions planned for their development.

The additional material: TUHAT compilation of the RC's other scientific activities/supervision of doctoral dissertations

A written feedback from the aspects of: processes and good practices related to leadership and management

- Strengths
- Areas of development
- Other remarks
- Recommendations

Numeric evaluation: OUTSTANDING (5), EXCELLENT (4), VERY GOOD (3), GOOD (2), SUFFICIENT (1)

### 3. The societal impact of research and doctoral training

- Description on how the RC interacts with and contributes to the society (collaboration with public, private and/or 3rd sector).
- Identification of the ways to strengthen the societal impact of the RC's research and doctoral training.

The additional material: TUHAT compilation of the RC's other scientific activities.

A written feedback from the aspects of: societal impact, national and international collaboration, innovativeness

- Strengths
- Areas of development
- Other remarks
- Recommendations

Numeric evaluation: OUTSTANDING (5), EXCELLENT (4), VERY GOOD (3), GOOD (2), SUFFICIENT (1)



#### **4. International and national (incl. intersectoral) research collaboration and researcher mobility**

- Description of
  - the RC's research collaborations and joint doctoral training activities
  - how the RC has promoted researcher mobility
- Identification of the RC's strengths and challenges related to research collaboration and researcher mobility, and the actions planned for their development.

A written feedback from the aspects of: scientific quality, national and international collaboration

- Strengths
- Areas of development
- Other remarks
- Recommendations

Numeric evaluation: OUTSTANDING (5), EXCELLENT (4), VERY GOOD (3), GOOD (2), SUFFICIENT (1)

#### **5. Operational conditions**

- Description of the operational conditions in the RC's research environment (e.g. research infrastructure, balance between research and teaching duties).
- Identification of the RC's strengths and challenges related to operational conditions, and the actions planned for their development.

A written feedback from the aspects of: processes and good practices related to leadership and management

- Strengths
- Areas of development
- Other remarks
- Recommendations

#### **6. Leadership and management in the researcher community**

- Description of
  - the execution and processes of leadership in the RC
  - how the management-related responsibilities and roles are distributed in the RC
  - how the leadership- and management-related processes support
    - high quality research
    - collaboration between principal investigators and other researchers in the RC
    - the RC's research focus
    - strengthening of the RC's know-how
- Identification of the RC's strengths and challenges related to leadership and management, and the actions planned for developing the processes

#### **7. External competitive funding of the RC**

- The RCs were asked to provide information of such external competitive funding, where:
  - the funding decisions have been made during 1.1.2005-31.12.2010, and
  - the administrator of the funding is/has been the University of Helsinki
- On the e-form the RCs were asked to provide:
  - 1) The relevant funding source(s) from a given list (Academy of Finland/Research Council, TEKES/The Finnish Funding Agency for Technology and Innovation , EU, ERC, foundations, other national funding organisations, other international funding organisations), and
  - 2) The total sum of funding which the organisation in question had decided to allocate to the RCs members during 1.1.2005-31.12.2010.

Competitive funding reported in the text is also to be considered when evaluating this point.

A written feedback from the aspects of: scientific quality, scientific significance, societal impact, innovativeness, future significance

- Strengths
- Areas of development
- Other remarks
- Recommendations

#### **8. The RC's strategic action plan for 2011-2013**

- RC's description of their future perspectives in relation to research and doctoral training.

A written feedback from the aspects of: scientific quality, scientific significance, societal impact, processes and good practices related to leadership and management, national and international collaboration, innovativeness, future significance

- Strengths
- Areas of development

- Other remarks
- Recommendations

## 9. Evaluation of the category of the RC in the context of entity of the evaluation material (1-8)

The RC's fitness to the chosen participation category

A written feedback evaluating the RC's fitness to the chosen participation category

- Strengths
- Areas of development
- Other remarks
- Recommendations

Numeric evaluation: OUTSTANDING (5), EXCELLENT (4), VERY GOOD (3), GOOD (2), SUFFICIENT (1)

## 10. Short description of how the RC members contributed the compilation of the stage 2 material

Comments on the compilation of evaluation material

## 11. How the UH's focus areas are presented in the RC's research?

Comments if applicable

## 12. RC-specific main recommendations based on the previous questions 1-11

## 13. RC-specific conclusions

# 1.7 Evaluation criteria

The panellists were expected to give evaluative and analytical feedback to each evaluation question according to their aspects in order to describe and justify the quality of the submitted material. In addition, the evaluation feedback was asked to be pointed out the level of the performance according to the following classifications:

- outstanding (5)
- excellent (4)
- very good (3)
- good (2)
- sufficient (1)

Evaluation according to the criteria was to be made with thorough consideration of the entire evaluation material of the RC in question. Finally, in questions 1-4 and 9, the panellists were expected to classify their written feedback into one of the provided levels (the levels included respective descriptions, 'criteria'). Some panels used decimals in marks. The descriptive level was interpreted according to the integers and not rounding up the decimals by the editors.

## Description of criteria levels

### Question 1 – FOCUS AND QUALITY OF THE RC'S RESEARCH

#### Classification: Criteria (level of procedures and results)

#### Outstanding quality of procedures and results (5)

Outstandingly strong research, also from international perspective. Attracts great international interest with a wide impact, including publications in leading journals and/or monographs published by leading international publishing houses. The research has world leading qualities. The research focus, key research questions scientific significance, societal impact and innovativeness are of outstanding quality.

*In cases where the research is of a national character and, in the judgement of the evaluators, should remain so, the concepts of "international attention" or "international impact" etc. in the grading criteria above may be replaced by "international comparability".*

Operations and procedures are of outstanding quality, transparent and shared in the community. The improvement of research and other efforts are documented and operations and practices are in alignment with the documentation. The ambition to develop the community together is of outstanding quality.

#### **Excellent quality of procedures and results (4)**

Research of excellent quality. Typically published with great impact, also internationally. Without doubt, the research has a leading position in its field in Finland.

Operations and procedures are of excellent quality, transparent and shared in the community. The improvement of research and other efforts are documented and operations and practices are to large extent in alignment with the documentation. The ambition to develop the community together is of excellent quality.

#### **Very good quality of procedures and results (3)**

The research is of such very good quality that it attracts wide national and international attention.

Operations and procedures are of very good quality, transparent and shared in the community. The improvement of research and other efforts are documented and operations and practices are to large extent in alignment with the documentation. The ambition to develop the community together is of very good quality.

#### **Good quality of procedures and results (2)**

Good research attracting mainly national attention but possessing international potential, extraordinarily high relevance may motivate good research.

Operations and procedures are of good quality, shared occasionally in the community. The improvement of research and other efforts are occasionally documented and operations and practices are to large extent in alignment with the documentation. The ambition to develop the community together is of good quality.

#### **Sufficient quality of procedures and results (1)**

In some cases the research is insufficient and reports do not gain wide circulation or do not have national or international attention. Research activities should be revised.

Operations and procedures are of sufficient quality, shared occasionally in the community. The improvement of research and other efforts are occasionally documented and operations and practices are to some extent in alignment with the documentation. The ambition to develop the community together is of sufficient quality.

### **Question 2 – DOCTORAL TRAINING**

### **Question 3 – SOCIETAL IMPACT**

### **Question 4 – COLLABORATION**

#### **Classification: Criteria (level of procedures and results)**

#### **Outstanding quality of procedures and results (5)**

Procedures are of outstanding quality, transparent and shared in the community. The practices and quality of doctoral training/societal impact/international and national collaboration/leadership and management are documented and operations and practices are in alignment with the documentation. The ambition to develop the community together is of outstanding quality. The procedures and results are regularly evaluated and the feedback has an effect on the planning.

#### **Excellent quality of procedures and results (4)**

Procedures are of excellent quality, transparent and shared in the community. The practices and quality of doctoral training/societal impact/international and national collaboration/leadership and management are documented and operations and practices are to large extent in alignment with the documentation. The ambition to develop the community together is of excellent quality. The procedures and outcomes are evaluated and the feedback has an effect on the planning.

#### **Very good quality of procedures and results (3)**

Procedures are of very good quality, transparent and shared in the community. The practices and quality of doctoral training/societal impact/international and national collaboration/leadership and

management are documented and operations and practices are to large extent in alignment with the documentation. The ambition to develop the community together is of very good quality.

#### **Good quality of procedures and results (2)**

Procedures are of good quality, shared occasionally in the community. The practices and quality of doctoral training/societal impact/international and national collaboration/leadership and management are documented and operations and practices are to large extent in alignment with the documentation. The ambition to develop the community together is of good quality.

#### **Sufficient quality of procedures and results (1)**

Procedures are of sufficient quality, transparent and shared in the community. The practices and quality of doctoral training/societal impact/international and national collaboration/leadership and management are occasionally documented and operations and practices are to some extent in alignment with the documentation. The ambition to develop the community together is of sufficient quality.

### **Question 9 – CATEGORY**

Participation category – fitness for the category chosen

The choice and justification for the chosen category below should be reflected in the RC's responses to the evaluation questions 1–8.

1. *The research of the participating community represents the international cutting edge in its field.*
2. *The research of the participating community is of high quality, but the community in its present composition has yet to achieve strong international recognition or a clear break-through.*
3. *The research of the participating community is distinct from mainstream research, and the special features of the research tradition in the field must be considered in the evaluation.* The research is of high quality and has great significance and impact in its field. However, the generally used research evaluation methods do not necessarily shed sufficient light on the merits of the research.
4. *The research of the participating community represents an innovative opening.* A new opening can be an innovative combination of research fields, or it can be proven to have a special social, national or international demand or other significance. Even if the researcher community in its present composition has yet to obtain proof of international success, its members can produce convincing evidence of the high level of their previous research.
5. *The research of the participating community has a highly significant societal impact.* The participating researcher community is able to justify the high social significance of its research. The research may relate to national legislation, media visibility or participation in social debate, or other activities promoting social development and human welfare. In addition to having societal impact, the research must be of a high standard.

#### **An example of outstanding fitness for category choice (5)<sup>5</sup>**

The RC's representation and argumentation for the chosen category were convincing. The RC recognized its real capacity and apparent outcomes in a wider context to the research communities. The specific character of the RC was well-recognized and well stated in the responses. The RC fitted optimally for the category.

- Outstanding (5)
- Excellent (4)
- Very good (3)
- Good (2)
- Sufficient (1)

The above-mentioned definition of outstanding was only an example in order to assist the panellists in the positioning of the classification. There was no exact definition for the category fitness.

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<sup>5</sup> The panels discussed the category fitness and made the final conclusions of the interpretation of it.

## 1.8 Timetable of the evaluation

The main timetable of the evaluation:

- |  |                       |
|--|-----------------------|
| 1. Registration                            | November 2010         |
| 2. Submission of self-evaluation materials | January–February 2011 |
| 3. External peer review                    | May–September 2011    |
| 4. Published reports                       | March–April 2012      |
| - University level public report           |                       |
| - RC specific reports                      |                       |

The entire evaluation was implemented during the university's strategy period 2010–2012. The preliminary results were available for the planning of the following strategy period in late autumn 2011. The evaluation reports will be published in March/April 2012. More detailed time schedule is published in the University report.

## 1.9 Evaluation feedback – consensus of the entire panel

The panellists evaluated all the RC-specific material before the meetings in Helsinki and mailed the draft reports to the evaluation office. The latest interim versions were on-line available to all the panellists on the Wiki-sites. In September 2011, in Helsinki the panels discussed the material, revised the first draft reports and decided the final numeric evaluation. After the meetings in Helsinki, the panels continued working and finalised the reports before the end of November 2011. The final RC-specific reports are the consensus of the entire panel.

The evaluation reports were written by the panels independently. During the editing process, the evaluation office requested some clarifications from the panels when necessary. The tone and style in the reports were not harmonized in the editing process. All the reports follow the original texts written by the panels as far as it was possible.

The original evaluation material of the RCs, provided for the panellists is attached at the end of the report. It is essential to notice that the exported lists of publications and other scientific activities depend how the data was stored in the TUHAT-RIS by the RCs.



## 2 Evaluation feedback

### 2.1 Focus and quality of the RC's research

- *Description of*
  - *the RC's research focus*
  - *the quality of the RC's research (incl. key research questions and results)*
  - *the scientific significance of the RC's research in the research field(s)*
- *Identification of the ways to strengthen the focus and improve the quality of the RC's research*

*ASPECTS: Scientific quality, scientific significance, societal impact, innovativeness*

The RC is focusing on research in medicinal chemistry in different fields of cancer, antibiotics, metabolics and GPCR. As a relative small group they have been being quite productive concerning paper and patents.

In these different fields they have achieved excellent/very good results that have been published in the leading journals in that field. The work has been successfully supported by many EU grants as well as different national sources. The international network has greatly been enhanced by these European and world-wide structures.

With the relative small size of the groups the potential overlap in the topics can be used in a greater extend to have a greater synergistic effect and even higher output. The RC could define their "spearhead" projects for this collaboration. In this respect, the potential for co-operations within the UH also existing in many parts, can still be enlarged. Interaction with industry, apparently very limited at present, should be encouraged both for scientific debate in the field and for training and funding opportunities.

**Numeric evaluation: 3.5 (Very good)**

### 2.2 Practises and quality of doctoral training

- *Organising of the doctoral training in the RC. Description of the RC's principles for:*
  - *recruitment and selection of doctoral candidates*
  - *supervision of doctoral candidates*
  - *collaboration with faculties, departments/institutes, and potential graduate schools/doctoral programmes*
  - *good practises and quality assurance in doctoral training*
  - *assuring of good career perspectives for the doctoral candidates/fresh doctorates*
- *Identification of the RC's strengths and challenges related to the practises and quality of doctoral training, and the actions planned for their development.*
- *Additional material: TUHAT compilation of the RC's other scientific activities/supervision of doctoral dissertations*

*ASPECTS: Processes and good practices related to leadership and management*

There is an excellent/good and well organized training program for the PhD students. The outlook for good positions is good although the general number of free position for excellent academics is limited. The teaching work-load for the PhD students as well as for the supervisors at different levels is not clear, but the impression seems that there may be an overload or misbalance of too much teaching giving a smaller part for research.

The overall duration of PhD studies seems generally too long as compared to international standards. This has been well identified in RC. The practice of the needed publications should be work-on to find a balanced adaption. The difficulty with a general judgment of number of publications, problems with impact factors etc. has largely been discussed in other work, but quality should always be better handled

than quantity. Based on the statistics tables provided, the quality indicators, such as MNCS, should still be improved.

With the different faculties there seems to be different PhD student programs. With a general core structure on a number of RCs or faculties and then different specialized course for the detailed problems of the RC the work-load may be reduced and the outcome increased. A template or RC specific set of guidelines to outline a unified process and good practice and governance may be helpful for both doctorate candidates and supervisors.

**Numeric evaluation: 3 (Very good)**

## 2.3 The societal impact of research and doctoral training

- *Description on how the RC interacts with and contributes to the society (collaboration with public, private and/or 3rd sector).*
- *Identification of the ways to strengthen the societal impact of the RC's research and doctoral training.*
- *Additional material: TUHAT compilation of the RC's other scientific activities.*

**ASPECTS: Societal impact, national and international collaboration, innovativeness**

The fields of cancer, GPCR as well of drug misuse have great impact on society and receive great interest. The efforts in achieving external recognition for the RC's work in drugs of misuse and illicit drugs should be elevated domestically and internationally and such investment of time may lead to additional sources of funding from various agencies (e.g. international sports agencies, forensic agencies). Since some antibiotics become ineffective against some bacteria etc. there is also an increasing need for new antibiotics which are rarely covered by pharmaceutical industry.

New findings in the main research topics may drastically change the therapy of different diseases and the health situation.

The RC has improved concerning the international exchange during the last evaluation period and this trend should be further worked out.

The output to non-scientific community and the communication may be increased to help on the general acceptance and understanding on the time-scale and money consumption with drug development.

Indicators of research excellence, such as post of academy professor, status for a center of excellence or successful ERC grants, should actively be strived for. Those would significantly improve the recognition of RC.

**Numeric evaluation: 3 (Very good)**

## 2.4 International and national (incl. intersectoral) research collaboration and researcher mobility

- *Description of*
  - *the RC's research collaborations and joint doctoral training activities*
  - *how the RC has promoted researcher mobility*
- *Identification of the RC's strengths and challenges related to research collaboration and researcher mobility, and the actions planned for their development.*

**ASPECTS: Scientific quality, national and international collaboration**

The RC has improved the international exchange during the last evaluation period and this trend should be further worked out.

Numerous exchange programs are performed with other European countries. The full potential of short termed exchange missions within COST or other programs has not been taken full advantage. The potential for UH co-operations can also to be increased as some connections are striking with the inspection of different RCs.



PhD student exchange from and to UH may be increased to get a higher level of international exchange in information and needed instrumentation.

**Numeric evaluation: 3 (Very good)**

## 2.5 Operational conditions

- *Description of the operational conditions in the RC's research environment (e.g. research infrastructure, balance between research and teaching duties).*
- *Identification of the RC's strengths and challenges related to operational conditions, and the actions planned for their development.*

**ASPECTS: Processes and good practices related to leadership and management**

Administrative work and teaching duties seem to take a lot of time from research. It may have some advantage to have an effective administration asking the researchers what they can do for them and in which way administration may help the researchers. Quite often the administration has developed and increased themselves with higher bureaucracy etc. With the development of new administrative structures the ways may have get longer instead of shorter and more direct/problem oriented. This does not seem to be specific for this RC, it seems to be a more or less general problem with all universities.

The RC is linked to two administrative units – Division of Pharmaceutical Chemistry and the Centre for Drug Research. It is not clear, what are the relationships between the RC and these units in terms of governance and management.

## 2.6 Leadership and management in the researcher community

- *Description of*
  - *the execution and processes of leadership in the RC*
  - *how the management-related responsibilities and roles are distributed in the RC*
  - *how the leadership- and management-related processes support*
    - *high quality research*
    - *collaboration between principal investigators and other researchers in the RC*
    - *the RC's research focus*
    - *strengthening of the RC's know-how*
- *Identification of the RC's strengths and challenges related to leadership and management, and the actions planned for developing the processes*

**ASPECTS: Processes and good practices related to leadership and management**

Despite a clear hierarchy the RC is led by a team consisted of the group leaders. They show together concerted actions and friendly agreement with decisions. Within the university, Division of Pharmaceutical Chemistry/DPC and Centre for Drug Research/CDR is not an easy task to discriminate different groups or research topics.

Nevertheless, some more general guidelines for cooperative decision-making within the teams (fixed meeting dates, RC's research area sharpening, equipment etc.) in organizational aspects as well as in case of conflicts may be useful. In this respect some more time of RC members in the general management would be useful which may be dampened by the workload with teaching and bureaucracy.

The leadership role can be improved by UH or Finnish workshops on RC immanent topics as well as with an application within a larger consortium having one of the leading positions within the next few years.

## 2.7 External competitive funding of the RC

- *The RCs were asked to provide information of such external competitive funding, where:*
  - *the funding decisions have been made during 1.1.2005–31.12.2010, and*
  - *the administrator of the funding is/has been the University of Helsinki*
- *On the e-form the RCs were asked to provide:*
  - 1) *The relevant funding source(s) from a given list (Academy of Finland/Research Council, TEKES/The Finnish Funding Agency for Technology and Innovation, EU, ERC, foundations, other national funding organisations, other international funding organizations), and*
  - 2) *The total sum of funding which the organisation in question had decided to allocate to the RCs members during 1.1.2005–31.12.2010.*

*Competitive funding reported in the text is also to be considered when evaluating this point.*

*ASPECTS: Scientific quality, scientific significance, societal impact, innovativeness and future significance*

The RC made an excellent external funding with huge amounts of money for this community size (in total about 4 M€) which is above the usual budget for this kind of research. It shows the string competitive character of the group within the international scientific community. The diverse structure from national and international sources put this on a broad position.

## 2.8 The RC's strategic action plan for 2011–2013

- *RC's description of their future perspectives in relation to research and doctoral training.*

*ASPECTS: Scientific quality, scientific significance, societal Impact, processes and good practices related to leadership and management, national and international collaboration, innovativeness, future significance*

The interdisciplinary approach on many topics is highly appreciated.

The focus on the overlap of existing projects seems to highly useful for the next period. Some tight scientific connections to other RCs may be underestimated so far and need further inspection (e.g. HYRL, BNMTI, MAC etc.).

The cooperation with the other related organizations and RCs should be defined.

## 2.9 Evaluation of the category of the RC in the context of entity of the evaluation material (1-8)

*The RC's fitness to the chosen participation category.*

*Category 4. The research of the participating community represents an innovative opening.*

The RC is one of the national leading research teams in Medicinal Chemistry. It has achieved good internationalization and output in form of paper and patents. The innovative character has highly increased within the last evaluation period.

Within the relative small RC size they have achieved high output and very good visibility. The positive trend for research excellence is advancing.

The chosen category is well taken although other possibilities may also be considered with the further focus in research.

**Numeric evaluation: 4 (Excellent)**

## **2.10 Short description of how the RC members contributed the compilation of the stage 2 material**

The processes employed were fair and appropriate.

## **2.11 How the UH's focus areas are presented in the RC's research**

*Focus area 1: the basic structure, materials and natural resources of the physical world*

It was obvious from the presentation that MEDCHEMBIO belongs to several focus areas due its multidisciplinary in life sciences. The relevant focus areas are covered by the chosen scientific fields of the RC.

## **2.12 RC-specific main recommendations**

The clear advantage for more focused and condensed research areas within this rather small RC can be seen.

The exchange of PhD students could be increased and thereby helping to increase the international visibility of this excellent RC.

## **2.13 RC-specific conclusions**

The RC already has a high level of local, domestic and international co-operations and network. Additional approaches for further industrial contacts may help to take translational steps in research.

## **2.14 Preliminary findings in the Panel-specific feedback**

The RC has performed excellent to good research in different fields of medicinal chemistry with a slightly too high number of different topics/targets.

The doctoral training is well-organized and introduced in different doctoral programs. Any overlap in teaching may here be reduced by the reorganization of strongly related teaching stuff. The outcome for society is excellent with these highly educated valuable scientists with a very good to excellent international network.

Nationally they have achieved a good leadership position, but the clear role to the different research units have still to be defined and some breakthrough findings are to be awaited.

With the small size of the group they have achieved a broad and diverse funding at a very high level.

With the plans for the future an additional sharpening of the foci would help to drive the high potential of the RC into new findings and may be into further translational steps for drug development.

## **2.15 Preliminary findings in the University-level evaluation**

The RC has focused in different fields of medicinal chemistry. Some overlap in some topics of other RCs has been identified which may broaden the possibilities to study some to the focused topics into more details and at an even higher scientific level. These co-operations may then be used to take additional steps for drug development or metabolism studies for translational research.

The studies in these fields of life sciences have great societal impact.

The national and international network is already at a high level. Further stress into the broadening of this may have advantages for the exchange of PhD students and the international visibility.

The external funding is at an excellent level for this size of RC. This is especially true since funding for such basic and essential topics are usually difficult to find.

The strategic plan is a continuation of the previously successful research. The advantage of thematic overlap within the RC and within other local RC could strengthen the performance of the group as well as that of its (new) partners.

The group has published in the leading journals in this field and has taken some patents for further development. The networking within the scientific community of UH and of Finland in this life sciences needs further enhancement as the need and the demand for success is very high in this area.

# 3 Appendices

- A. Original evaluation material
  - a. Registration material – Stage 1
  - b. Answers to evaluation questions – Stage 2
  - c. List of publications
  - d. List of other scientific activities
- B. Bibliometric analyses
  - a. Analysis provided by CWTS/University of Leiden
  - b. Analysis provided by Helsinki University Library (66 RCs)



International evaluation of research and doctoral training  
at the University of Helsinki 2005-2010

RC-SPECIFIC MATERIAL FOR THE PEER REVIEW

NAME OF THE RESEARCHER COMMUNITY:

Medicinal Chemistry and Biochemistry Research Group (MEDCHEMBIO)

LEADER OF THE RESEARCHER COMMUNITY:

Professor Jari Yli-Kauhaluoma, Faculty of Pharmacy

RC-SPECIFIC MATERIAL FOR THE PEER REVIEW:

- Material submitted by the RC at stages 1 and 2 of the evaluation
  - STAGE 1 material: RC's registration form (incl. list of RC participants in an excel table)
  - STAGE 2 material: RC's answers to evaluation questions
- TUHAT compilations of the RC members' publications 1.1.2005-31.12.2010
- TUHAT compilations of the RC members' other scientific activities 1.1.2005-31.12.2010
- Web of Science(WoS)-based bibliometrics of the RC's publications data 1.1.2005-31.12.2010 (analysis carried out by CWTS, Leiden University)

*NB! Since Web of Science(WoS)-based bibliometrics does not provide representative results for most RCs representing humanities, social sciences and computer sciences, the publications of these RCs will be analyzed by the UH Library (results available by the end of June, 2011)*



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RC-SPECIFIC STAGE 1 MATERIAL (registration form)

1 RESPONSIBLE PERSON

Name: Yli-Kauhaluoma, Jari

E-mail:

Phone: 09-19159170

Affiliation: Professor, Head of Division, Vice-director of the GS in Pharmaceutical Research

Street address: Faculty of Pharmacy, Division of Pharmaceutical Chemistry, Viikinkaari 5 E (PO Box 56),  
00014 University of Helsinki

2 DESCRIPTION OF THE PARTICIPATING RESEARCHER COMMUNITY (RC)

Name of the participating RC (max. 30 characters): Medicinal Chemistry and Biochemistry Research Group

Acronym for the participating RC (max. 10 characters): MEDCHEMBIO

Description of the operational basis in 2005-2010 (eg. research collaboration, joint doctoral training activities) on which the RC was formed (MAX. 2200 characters with spaces): The Medicinal Chemistry and Biochemistry Research Group (MEDCHEMBIO), combines the medicinal chemistry-related research efforts of four principal investigators of the Faculty of Pharmacy in a coherent and complementary manner. The focus is medicinal chemistry, which is a chemistry-based discipline, also involving aspects of biological, medical and pharmaceutical sciences. Medicinal chemistry is concerned with the invention, discovery, design, identification and preparation of biologically active compounds, the study of their metabolism, the interpretation of their mode of action at the molecular level and the construction of structure-activity relationships.

The principal investigators and their key expertise are Dr. Moshe Finel (research group leader, docent of medical chemistry, research focus biochemistry of drug metabolism), Dr. Erik Wallén (research group leader, docent of medicinal chemistry, research focus synthesis of peptidomimetics), Dr. Henri Xhaard (research group leader, research focus computer-aided drug design and cheminformatics) and Dr. Jari Yli-Kauhaluoma (professor of medicinal chemistry, research group leader, research focus medicinal, organic and natural product chemistry).

All the principal investigators of the MEDCHEMBIO researcher community have collaborated with each other during the evaluation period and, between them, have been in charge of joint doctoral training and supervision of 22 PhD students, as well as involved in the supervision of 9 PhD students not belonging to this RC. The combined research activity of the RC members yielded 112 scientific articles and 5 PhD degrees during 2005-2010.



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3 SCIENTIFIC FIELDS OF THE RC

Main scientific field of the RC's research: natural sciences

RC's scientific subfield 1: Chemistry, Medicinal

RC's scientific subfield 2: Pharmacology and Pharmacy

RC's scientific subfield 3: Chemistry, Organic

RC's scientific subfield 4: Biochemistry and Molecular Biology

Other, if not in the list:

4 RC'S PARTICIPATION CATEGORY

Participation category: 4. Research of the participating community represents an innovative opening

Justification for the selected participation category (MAX. 2200 characters with spaces): The MEDCHEMBIO researcher community combines various disciplines, such as pharmaceutical sciences, organic chemistry, biochemistry, molecular biology, theoretical and computational chemistry as well as biology in its research.

The MEDCHEMBIO group started its research projects with a focus on the discovery of new bioactive compounds and study of their metabolism, particularly glucuronidation, in 2004 with two principal investigators (the number of principal investigators increased to three in 2007 and to four in 2008). Noteworthy, the first professorship in medicinal chemistry at the University of Helsinki was established in the Faculty of Pharmacy in 2006, and it is the only professorship in synthetic medicinal chemistry in the whole country.

The various research projects of the MEDCHEMBIO group have resulted in 112 publications in high-quality journals (e.g. J. Med. Chem., DMD, Mol. Pharmacol., Org. Lett.) and 6 patent applications during the evaluation period, an indication of the innovation of the MEDCHEMBIO group.

The laboratories that participate in this group have developed new methodologies that were not available at the University of Helsinki before, such as combinatorial chemistry, peptidomimetics, full set of 19 human UDP-glucuronosyltransferase enzymes for glucuronidation studies, GPCR modeling, studies of semisynthetic natural compounds as antimicrobial and antiviral agents, as well as design and synthesis of compounds targeted at protein kinases. An additional strength of the MEDCHEMBIO is that the key activities in computer-aided methods, synthesis and biochemistry are present in the same researcher community. These lines of research are all integral part of modern drug discovery and add important new possibilities for both researchers and doctoral training.

5 DESCRIPTION OF THE RC'S RESEARCH AND DOCTORAL TRAINING

Public description of the RC's research and doctoral training (MAX. 2200 characters with spaces): The Medicinal Chemistry and Biochemistry Research Group (MEDCHEMBIO) has been focusing on drug





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discovery and on applying and developing methods in medicinal chemistry, particularly synthetic organic chemistry, molecular modelling and drug metabolism. The MEDCHEMBIO group is the only group at the University that is translating the increasing structural information of drug targets or ligands (biologically active natural compounds or peptides) into the synthesis of small molecular weight compounds that are original and unavailable from current commercial compound libraries.

The research of the group is focused on chemotherapeutics, mainly against cancer (kallikreins and protein kinases, such as PKC, ALK, Pim) but also against intracellular pathogenic bacteria (Chlamydia), alphaviruses and parasites (Leishmania). The compounds serve, or will serve, as probes in the research of new drug targets and as hits or leads in the search for new therapeutic compounds. Moreover, the methodologies used by the group have a wide general applicability and could be applied to other types of projects, beyond medicinal chemistry, such as chemical biology and more. For example, the biologically active compounds can be used as specific probes for studying the biochemical function or cellular localization of enzymes and other proteins.

The metabolism studies of the MEDCHEMBIO group incorporate steroid metabolism and UDP-glucuronosyltransferases (UGTs) research, which is mainly centered on the glucuronidation of drugs and endogenous compounds. The group has an internationally unique source of all the 19 human UGTs as recombinant proteins. The UGTs research and gained expertise are also at the basis of several productive scientific collaborations and the success of this research direction efficiently links various research teams beyond MEDCHEMBIO.

The research in the MEDCHEMBIO group has resulted in 5 PhD degrees during the evaluation period. Doctoral training is closely linked to the Graduate School in Pharmaceutical Research and National GS in Informational and Structural Biology. We are also actively collaborating with the GS in Organic Chemistry and Chemical Biology.

Significance of the RC's research and doctoral training for the University of Helsinki (MAX. 2200 characters with spaces): The Medicinal Chemistry and Biochemistry Research Group contributes to the joint research efforts and doctoral training of the University of Helsinki in several ways. It provides a unique combination of scientific expertise in medicinal chemistry with three different main lines: synthetic medicinal chemistry, computational medicinal chemistry and drug metabolism, bridging academic and industrial drug discovery and development.

The MEDCHEMBIO group has established a close collaboration with many domestic and international research groups that are active in biological screening and research of new drug targets. It also coordinates and participates in various European Community-funded projects and research networks, such as Protein Kinase Research, LIINTOP, FORESTSPECS, MAREX and the COST Programme "New drugs for neglected diseases" among others. We have gained valuable experience in these highly collaborative, multidisciplinary and international projects both as coordinators and as active contributors.

Finally, the MEDCHEMBIO group focuses on several aspects of drug discovery and the group is applying and developing methods in modern medicinal chemistry, most importantly synthetic organic chemistry, molecular modelling, and drug metabolism. The MEDCHEMBIO is the only group at the University of



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Helsinki that combines synthetic, computational and biochemical methods in medicinal chemistry and translates the increasing structural information of drug targets or ligands into new, small molecular weight compounds.

Keywords: medicinal chemistry, drug discovery, drug metabolism, molecular modelling, organic synthesis, pharmacy

6 QUALITY OF RC'S RESEARCH AND DOCTORAL TRAINING

Justified estimate of the quality of the RC's research and doctoral training at national and international level during 2005-2010 (MAX. 2200 characters with spaces): A part of the current MEDCHEMBIO group (Wallén and Yli-Kauhaluoma) conducted a benchmarking self-assessment of the quality of their research and doctoral training at national and international levels for the Evaluation of Chemistry Research in Finland by the Academy of Finland in 2010. For that evaluation we had to suggest a reference unit and, rather than selecting a "regular" chemistry department, we suggested the Division of Medicinal Chemistry (DMC) at the Vrije Universiteit from the internationally highly-ranked Leiden/Amsterdam Center for Drug Research, as a reference for that self-evaluation exercise. Both our and the DMC units conduct medicinal chemistry research in similar environment of biological and pharmaceutical sciences and, therefore, the DMC is a very good group to compare to.

The DMC in Amsterdam mainly approaches medicinal chemistry from the pharmacological perspective, while our group has strong organic chemistry and biochemical points of view. The number of our personnel is less than half of DMC's, with the notable exception of the number of PIs, that being in Helsinki one-third of the Amsterdam's DMC. Nevertheless, despite having less resources and being a significantly younger research group, our team has succeeded in publishing its key findings in similar level of scientific journals as the DMC unit. We have published some of its chemistry research even in higher-ranking journals than the DMC unit. For example, we had three articles in Organic Letters during the evaluation period, actually representing 21% of all the Finnish articles in this highest impact journal in the field of organic chemistry.

N.B. The Academy of Finland evaluation was focused on the administratively defined chemistry units rather than the current evaluation of the Researcher Communities and this is why the research groups of PIs Finel and Xhaard were not part of that. The latter groups are members of the current RC for the University of Helsinki evaluation and the many additional publications of theirs were not included in the chemistry evaluation, but will be included in the current evaluation.

Comments on how the RC's scientific productivity and doctoral training should be evaluated (MAX. 2200 characters with spaces): We intend to use Leiden/Amsterdam Center for Drug Research for scientific "benchmarking" and self-evaluation purposes in the future, particularly if it maintains or improves its internationally high scientific level. The self-evaluation forms may serve as the basis for assessing the MEDCHEMBIO's scientific productivity and doctoral training, once the contributions of the laboratories of Moshe Finel and Henri Xhaard that did not participate in the chemistry evaluation, have been added. The selection of the Dutch unit is supported by a thorough bibliometric analysis, including factors such as (i) the number of publications by the principal investigators during the evaluation period according to ISI Web of



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RC-SPECIFIC STAGE 1 MATERIAL (registration form)

Knowledge, (ii) the number of citations to these publications, (iii) average citations per item, and (iv) the group's h-index. Other important factors are the quantity (number) and quality (grades, prizes) of the PhD theses finalized during the evaluation period, as well as the present employment of the graduated PhDs from the MEDCHEMBIO group. Assessing the innovativeness of the MEDCHEMBIO group, another important topic, should take into account submitted patent applications and granted patents. Finally, the quality of education, supervision and leadership practices of the MEDCHEMBIO doctoral training should be taken into account.

The research results of the MEDCHEMBIO group projects have been and will be published in peer-reviewed international scientific journals and in international scientific conference proceedings (posters and oral presentations). The aim is to submit the manuscripts to the most appropriate journals in the field. Most influential journals of medicinal chemistry and drug metabolism are Journal of Medicinal Chemistry (impact factor 4.802) and Journal of Chemical Information and Modeling (IF 3.882) by the American Chemical Society's as well as Drug Metabolism and Disposition (IF 3.743), Molecular Pharmacology (IF 4.531) and Journal of Pharmacology and Experimental Therapeutics (IF 4.093) by the American Society for Pharmacology and Experimental Therapeutics. If appropriate, Finnish and/or international patent applications will be filed.

## LIST OF RC MEMBERS

NAME OF THE RESEARCHER COMMUNITY:			Medicinal Chemistry and Biochemistry Research Group (MEDCHEMBIO)		
RC-LEADER			J. Yli-Kauhaluoma		
Category			4		
	Last name	First name	PI-status (TUHAT, 29.11.2010)	Title of research and teaching personnel	Affiliation
1	Finel	Moshe	x	university researcher	Faculty of Pharmacy
2	Wallén	Erik	x	university lecturer	Faculty of Pharmacy
3	Xhaard	Henri	x	university researcher	Faculty of Pharmacy
4	Yli-Kauhaluoma	Jari	x	university researcher	Faculty of Pharmacy
5	Aumüller	Ingo		postdoctoral researcher	Faculty of Pharmacy
6	Harju	Kirsi		doctoral candidate - postdoctoral researcher	Faculty of Pharmacy
7	Kiuru	Paula		postdoctoral researcher	Faculty of Pharmacy
8	Laakkonen	Liisa		senior researcher	Faculty of Pharmacy
9	Rajaratnam	Mohanathas		postdoctoral researcher	Faculty of Pharmacy
10	Regad	Leslie		postdoctoral researcher	Faculty of Pharmacy
11	Samanta	Swapn		postdoctoral researcher	Faculty of Pharmacy
12	Tadd	Andrew		postdoctoral researcher	Faculty of Pharmacy
13	Alakurtti	Sami		doctoral candidate	Faculty of Pharmacy
14	Alkio	Martti		doctoral candidate	Faculty of Pharmacy
15	Bichlmaier	Ingo		doctoral candidate	Faculty of Pharmacy
16	Boije af Gennäs	Gustav		doctoral candidate	Faculty of Pharmacy
17	Haavikko	Raisa		doctoral candidate	Faculty of Pharmacy
18	Kaivosaaari	Sanna		doctoral candidate	Faculty of Pharmacy
19	Keurulainen	Leena		doctoral candidate	Faculty of Pharmacy
20	Kiriazis	Alexandros		doctoral candidate	Faculty of Pharmacy
21	Kurkela	Mika		doctoral candidate	Faculty of Pharmacy
22	Leikoski	Tuomo		doctoral candidate	Faculty of Pharmacy
23	Manevski	Nenad		doctoral candidate	Faculty of Pharmacy
24	Meinander	Kristian		doctoral candidate	Faculty of Pharmacy
25	Siiskonen	Antti		doctoral candidate	Faculty of Pharmacy
26	Sipilä	Julius		doctoral candidate	Faculty of Pharmacy
27	Sneitz	Nina		doctoral candidate	Faculty of Pharmacy
28	Sten	Taina		doctoral candidate	Faculty of Pharmacy
29	Stepniewski	Michal		doctoral candidate	Faculty of Pharmacy
30	Vahermo	Mikko		doctoral candidate	Faculty of Pharmacy
31	Wissel	Gloria		doctoral candidate	Faculty of Pharmacy
32	Zhang	Hongbo		doctoral candidate	Faculty of Pharmacy
33	Zhang	Yuezhou		doctoral candidate	Faculty of Pharmacy



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RC-SPECIFIC STAGE 2 MATERIAL

BACKGROUND INFORMATION

Name of the RC's responsible person: Yli-Kauhaluoma, Jari

E-mail of the RC's responsible person:

Name and acronym of the participating RC: Medicinal Chemistry and Biochemistry Research Group,  
MedChemBio

The RC's research represents the following key focus area of UH: 1. MaaIlman perusrakenne, materiaalit ja luonnonvarat – The basic structure, materials and natural resources of the physical world

Comments for selecting/not selecting the key focus area: The key words of the MedChemBio researcher community directly related to the selection of the selected key focus areas are medicinal chemistry, drug metabolism, drug discovery, computational modelling, chemoinformatics, chemistry, biology, medicines. This is why we have chosen both "The basic structure, materials and natural resources of physical world" and "Welfare and safety" as our key focus areas from the University list.

1 FOCUS AND QUALITY OF RC'S RESEARCH (MAX. 8800 CHARACTERS WITH SPACES)

- **Description of the RC's research focus, the quality of the RC's research (incl. key research questions and results) and the scientific significance of the RC's research for the research field(s).**

The main foci of RC are 1. Design, synthesis & biological evaluation of new compounds and modifications of known compounds leading to improved understanding of their structure-activity relationships (SAR); 2. Molecular biological studies to improve understanding of compounds recognition and drug metabolism; 3. Computational studies to provide fresh insight into SAR of compound series that are of current general interest or other available data that advance medicinal chemistry knowledge; 4. Studying the influence of compounds and proteins structure on biotransformation and pharmacokinetics; 5. Education of highly qualified researchers for both academia and industry.

Description of the RC research:

1. Cancer chemotherapy is one of the RC's main themes and our research has been focused on protein kinases and kallikreins. In EC and Academy of Finland (AF)-funded projects we have developed inhibitors for protein kinase C (PKC) isoenzymes, particularly new regulatory domain-targeted compounds. This led to the discovery of isophthalates as a new class of ligands affecting PKC activation with antiproliferative effects. Our PKC catalytic domain compounds combine inhibitory activity and cell penetration ability in a single molecule. We have supplied the ProKinase Consortium Library with >400 kinase-targeted in-house compounds and synthesized analogs of bistramide A (PKC-modulating natural compound) together with P. Goekjian. The collaboration with L. Scapozza and C. Gambacorti resulted in a series of new and selective urea-based inhibitors targeted at the catalytic site of anaplastic lymphoma kinase. In collaboration with P. Koskinen we have discovered heptafulvenes and tropones as a new class of potent Pim family kinase inhibitors that efficiently block many Pim-dependent cellular functions. These cell-permeable pan-Pim inhibitors can be used not only as efficient research tools, but also as promising hits against tumors overexpressing Pim kinases.

The human kallikreins (KLK) are a family of 15 closely related serine proteases. In addition to other roles, KLK3 has an antiangiogenic effect. There are few peptides that have the unique biological activity of stimulating KLK3 and we are interested in developing peptidomimetics of these peptides. An AF-funded project was started by studying the most active bicyclic peptide made up of 13 amino acids with two disulfide bridges. The non-terminal disulfide bridge was first investigated by replacing it with different



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### RC-SPECIFIC STAGE 2 MATERIAL

hydrocarbon cross linkers. As a first result, the synthetic routes to the cross linkers have been published. The final aim is to transfer the peptide into a non-peptidic scaffold. The most important collaborator is K. Luthman. The computational part of the project is performed in collaboration with A. Poso. The RC is also using structural bioinformatics for peptide modeling and to identify privileged chemical structures among inhibitors of serine proteases.

2. New bioactive compounds against intracellular pathogens. With financial support from EC, Tekes and many foundations we have explored betulin, a main terpene constituent of the birch bark waste of a forest industry, as a starting material for pharmaceutical applications. The main results, in collaboration with C. Jaffe, K. Janda, P. Vuorela and P. Tammela, have been the discovery of semisynthetic betulin derivatives as antimicrobial agents against various intracellular pathogens and viruses, such as *L. donovani*, *C. botulinum*, *C. pneumoniae* and alphaviruses. We have also designed and synthesized 2-aryl benzimidazoles that inhibit the growth of Chlamydiae. Another line of forest waste research, funded by Forestcluster, has resulted in abietane derivatives inhibiting growth of Leishmania parasites and preventing formation of Staphylococcus biofilms. Computational methods have been used to study SAR of these compounds and to construct a related chemogenomic map of diseases and targets.

3. Metabolism of drugs, other xenobiotics and lipophilic endogenous compounds. We have been cloning, expressing and studying the human UDP-glucuronosyltransferase enzymes (UGTs) to gain better understanding of human drug metabolism and related processes. These enzymes catalyze the conjugation of many drugs and other small lipophilic molecules with glucuronic acid, thereby often inactivating them and stimulating their excretion from the body. We have a unique collection of 19 human UGTs as recombinant proteins and use them for multiple studies, such as on substrate specificity of individual UGTs. In these studies we also employ compounds synthesized in the RC, such as the high selectivity inhibitors of individual UGTs. Among our main research topics have also been the glucuronidation of steroids and extrahepatic drug glucuronidation. Computational models of UGTs structure, active sites and substrate binding are currently being developed. Our UGTs research, enzymes and mutants have been the basis of productive scientific collaborations with different laboratories, both domestic and international. The major funding has been from UH, AF, EC, Juselius Foundation and GSPR.

4. G protein-coupled receptors (GPCRs) are an important class of drug targets and 40% of drugs currently on the market are targeted at them. Funding from UH was obtained, in collaboration with J. Kukkonen, for developing compounds active toward the orexin receptors. The RC has developed compounds active at the alpha-2 adrenergic receptors in collaboration with M. Scheinin. Efforts have also been made to develop new computational tools and assess existing tools, supported by ISB Graduate School.

During 2005-10 our RC has published 112 scientific articles in international peer-reviewed journals. Our research has yielded 1 patent and 8 patent applications, and we have supervised 5 completed PhD degrees. We have been in charge of supervision of a total of 22 PhD students (incl. the completed studies) and involved in supervision of 9 PhD students not belonging to this RC. We have published our research in journals such as *J. Med. Chem.*, *Org. Lett.*, *Mol. Pharmacol. & Drug Metab. Dispos.*, all among the top journals in the field. The RC members have given many presentations in international meetings. We have been particularly successful in obtaining highly-competed EC and AF funding for our research, the respective shares of the total RC external funding being 33% and 23%.

For self evaluation of our research, we have been using the Division of Medicinal Chemistry (DMC) from the internationally high-ranked Leiden/Amsterdam Center for Drug Research as a reference point. Both we and them conduct medicinal chemistry research in a similar environment of biological and pharmaceutical sciences and not, for example, in chemistry departments of the respective universities. The following is bibliometric data of DMC and our RC during 2005-10, respectively: number of articles 114, 112; citations to articles 1741, 811; h-index based on the articles 21, 16; and average citation per



## INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE UNIVERSITY OF HELSINKI

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item 15.27, 7.24. According to these parameters, the quality of our RC research starts to approach that of the DMC. This is despite having significantly less resources and being a significantly younger team. Noteworthy, we have published our research results and finding in similar type of scientific journals as the DMC.

We recently participated in the evaluation of Finnish chemistry research that was conducted by the AF. The international evaluation panel has concluded its report (<http://tinyurl.com/67ccht1>) saying that "The unit should maintain its research direction and level of achievement, which is of high quality in an important societal area."

- **Ways to strengthen the focus and improve the quality of the RC's research.**

RC's strengths are: 1. The RC combines complementary expertise of two units within the Faculty. 2. Our methodologies can be applied to other types of projects beyond medicinal chemistry such as chemical biology, and for studying biochemical function and cellular localization of enzymes and receptors. 3. All our PI's have spent >2 years in leading research groups abroad, and promote open collaborative scientific work. 4. None of the PI's has been recruited in-house, the typical drawback wherein the faculty members are recruited among their own alumni.

The quality of our research is likely to improve by the following actions: 1. Annual self-evaluation of scientific progress, productivity and quality by using the internationally recognized Dutch DMC as a reference unit. 2. Recruitment of more post-doctoral researchers (if suitable funds are available). 3. The EC-funded MAREX project will generate new scientific collaborations and research into bioactive marine compounds. 4. Locally, the Biocenter Finland network is likely to further stimulate collaborations with medical researchers.

#### 2 PRACTISES AND QUALITY OF DOCTORAL TRAINING (MAX. 8800 CHARACTERS WITH SPACES)

- How is doctoral training organised in the RC? Description of the RC's principles for recruitment and selection of doctoral candidates, supervision of doctoral candidates, collaboration with faculties, departments/institutes, and potential graduate schools/doctoral programmes, good practises and quality assurance in doctoral training, and assuring good career perspectives for the doctoral candidates/fresh doctorates.

Recruitment: The majority of the RC doctoral student positions are announced in the Recruitment web page of the University. The PI's review the applications that are treated in equal manner during the evaluation and selection process. A completed MSc degree is the first criterion for the applicants of doctoral student positions. The other selection criteria are the scientific quality of a research plan, previous scientific achievements of the applicant and the probability that the candidate will successfully complete his/her doctoral studies within a reasonable time. Recruitment is based on the guidelines of the Ministry of Education and Culture, and participation of younger and female doctoral students is encouraged. The top candidates are interviewed by the PI's.

Supervision of doctoral candidates: The objective of supervision is to commit doctoral candidates to the completion of their PhD degree and to commit the University, Faculty and the RC to the provision of the necessary teaching, supervision and support. Special attention is paid to supervision at the initial stage of doctoral studies. Doctoral candidates are provided with orientation to doctoral studies and are guided in making good use of the available course offerings. Student integration into the scholarly community is also promoted. The Faculty Council has approved guidelines concerning the rights and duties of supervisors and doctoral students. When making supervision arrangements, the doctoral students and their supervisors are expected to study these guidelines ("Supervisory expectations and responsibilities").



## INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE UNIVERSITY OF HELSINKI

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The supervisor and doctoral student meet regularly to assess progress in research and doctoral studies. The supervision is more intense at the beginning of doctoral studies, while more responsibility is given to the doctoral student at later stages with aim of “generating” an independent and critically thinking scientist of him/her. All the research groups of the RC organize regular group meetings where the research-related issues are discussed. Doctoral students can make alteration to their study plan with supervisor’s approval. If a research plan changes drastically or if a supervisor is changed, the Research Affairs Committee of the Faculty should approve the development. The doctoral students themselves have responsibility for their progress and must inform their supervisor and the Faculty if their studies are considerably delayed for some reason (e.g. maternity/parental leave, work circumstances).

Three instruments are used to guide the supervision of doctoral studies. First, the preliminary research plan is part of the application package when a person applies for the doctoral student position. The plan is based on the choice of a major subject at the start of the doctoral studies, and is drawn up with the supervisor’s assistance. Second, the personal study plan is based on the Faculty’s postgraduate application form, and doctoral students discuss their study plan (e.g. research schedule and content of studies, lecture and laboratory courses that support research) with their supervisor. Third, defence of the research proposal is required at 1–2 years after starting the doctoral studies. The doctoral students prepare the research plan and the supervisor comments on it before it is sent to the members of the evaluation board. The aim of the research plan defence is to evaluate how well a student can plan research, as well as to debate, defend and discuss the topics of his/her research. Essential and fundamental theoretical background of the research is also examined. Feedback from research plan defence is given to the doctoral student and his/her supervisors as a written report.

Collaboration with faculties, departments/institutes, and potential graduate schools/doctoral programmes: Our RC has direct links to the Graduate School in Pharmaceutical Research (GSPR), a national graduate school that was founded as collaboration between the University of Helsinki and the University of Eastern Finland (Kuopio) in 1998. Moreover, the current vice director of GSPR is the coordinator of our RC. GSPR is part of the FinPharmaNet network of Graduate Schools. It offers a multi-disciplinary and well-organized doctoral education in pharmaceutical research. It includes several research groups and is a part of national and international pharmaceutical research network including connections with pharmaceutical companies. GSPR grants travel funds for doctoral students that wish to visit foreign collaborating laboratories and carry out part of their research abroad. Our RC also has one doctoral student in the National Doctoral Program in Informational and Structural Biology, and good contacts with the National Graduate School of Organic Chemistry and Chemical Biology. Our RC is also part of the Paul Ehrlich MedChem Euro-PhD Network, the aim of which is to foster education and research training of post-graduate students in medicinal chemistry in Europe.

The RC has excellent contacts with the home faculty, Faculty of Pharmacy, as well as with other faculties and institutes in the Viikki Campus, and rest of the University of Helsinki. In particular, this includes the Faculties of Veterinary Medicine, Agriculture and Forestry, Science, Medicine, and the Institute of Biotechnology and the Neuroscience Centre. Moreover, the RC has an extensive domestic and international research network as described later.

Good practises and quality assurance in doctoral training: The doctoral training in our RC is mainly based on the rules, regulations and recommendations of the University, Faculty and GSPR. Quality at the University means expedient activity and high-quality results which is illustrated tangibly in, for example, the quality handbooks of the Faculty and GSPR (the operating procedures of the Division of Pharmaceutical Chemistry and Centre for Drug Research are described in the Quality Manuals of the respective units). The following is a brief collection of “good practises” at our RC: 1. Faculty





## INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE UNIVERSITY OF HELSINKI

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Postgraduate Study Guide; 2. clear and instructional web pages of the GSPR; 3. regular research group meetings; 4. personal study plans of doctoral students; 5. defence of the research proposal.

Assuring good career perspectives for the doctoral candidates/fresh doctorates: Our RC provides an excellent learning environment for postdoctoral fellows, postgraduate and undergraduate students. The variety of interdisciplinary pursuits with ambitious goals encompassed by our many projects ensures that they will gain expertise in a broad array of methodologies and techniques. Hence, they are well-poised to succeed as independent and highly competent scientists, either in industry or academia. These possibilities increase the likelihood of benefiting society, both as a result of the practical and theoretical capabilities of our fresh doctorates and postdoctoral fellows, as well as due to their abilities to teach and lead others. Nearly all the candidates who obtained their PhD or MSc degrees during the evaluation period have found their current employment that corresponds or is complementary to their doctoral training. Finally, our RC is one of the very few training places for students in chemoinformatics in Finland.

Our RC participated recently in the evaluation of the chemistry research in Finland 2005-9 by the Academy of Finland. The international evaluation panel concluded in their final report (<http://tinyurl.com/67ccht1>) that "The unit provides an excellent learning environment for postdoctoral fellows and postgraduate and undergraduate students."

- RC's strengths and challenges related to the practises and quality of doctoral training, and the actions planned for their development.

Strengths: (i) We have started to increase the exposure of undergraduate students to the scientific research in our laboratories by providing them a possibility and incentive to carry out part-time research work in the laboratory, alongside their regular studies. To this end we have established a course Laboratory Experience within a Research Group (3-5 cu). Four undergraduate students are currently involved in this activity in our RC. (ii) Our extensive national and international networks for doctoral training, as well as excellent scientific collaborators, are among the strengths of the RC. (iii) We have compiled a Postgraduate Handbook with good practises of doctoral training.

Challenges: (i) Obtaining the PhD degree takes still too long a time (>4 years), mostly due to short-term or dispersed funding by the funding agencies. Another possible reason for this is the "unwritten" requirement to include 4 peer-reviewed articles in PhD theses of the University of Helsinki. (ii) Another challenge is to stimulate the RC doctoral students to carry out part of their research abroad.

#### 3 SOCIETAL IMPACT OF RESEARCH AND DOCTORAL TRAINING (MAX. 4400 CHARACTERS WITH SPACES)

- Description of how the RC interacts with and contributes to the society (collaboration with public, private and/or 3rd sector).

Our interactions with the society are primarily realized via our research and researchers training. The following is a description of our societal impact and its public visibility.

First, we initiated negotiations among the Finnish medicinal chemistry community to join the European Federation of Medicinal Chemistry. As a result, Finland is now a full member of EFMC, whose objective is to advance the medicinal chemistry science by promoting cooperation, contacts and exchanges between European medicinal chemists.

Second, we participate in collaborative research with industry and SMEs. Such projects have been funded by EC, Tekes, pharmaceutical industry and Forestcluster (Finnish Strategic Centre for Science, Technology and Innovation). Many patent applications have been filed already (n=8), and researchers from industry (n=2) have visited us to learn and adopt new techniques while doing research for their



## INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE UNIVERSITY OF HELSINKI

### RC-SPECIFIC STAGE 2 MATERIAL

PhD degrees. Our RC has also played an active role in creating new research programs, such as Drug-2000 and IVIVRe, financed by the industry and Tekes.

Third, we belong to the Drug Discovery and Chemical Biology program for translational research of Biocenter Finland. We aim to provide advice and resources for development of chemical biology and its applications. We coordinate chemical compound databases, make our compounds available for virtual chemical screening and provide tools & scientific expertise.

Fourth, we carry out anti-doping, forensic and illicit drug research. 1. Our RC has participated in three World Anti-Doping Agency-funded projects and supplied the accredited doping control laboratories with reference substances worldwide (psychostimulant, steroid & antiestrogen metabolites). The reference substances enable reliable and legally defensible confirmation analysis of these drugs from the doping control samples. 2. Another WADA-supported research project was identification of the UGT enzymes that catalyze the glucuronidation of testosterone and epitestosterone, and clarification of genetic reasons that make testosterone and related steroids abuse by athletes from certain populations largely undetectable by the current approved method to test for such doping in major international sport competitions. Hence, our studies for WADA have contributed to curbing illicit athletes doping. 3. We have studied the glucuronidation of psilocin and identified UGTs that catalyze metabolic clearance of this hallucinogenic drug of abuse. This recent study is expected to facilitate forensic investigations of psilocin and related drugs. The extensive explorations we have done into drug glucuronidation will help to reduce adverse drug effects in humans, both by enabling more accurate dosing of individual drugs to individual patients, and by improving prevention of drug-drug interactions. Another societal contribution is a significant contribution to the quality and professionalism, in different aspects of medicinal chemistry and biotransformation, of employees in both pharmacies and in drug regulatory agencies in Finland.

Fifth, RC is publicly visible. We have given popular lectures of medicinal chemistry research to students and teachers in the local schools. Our research has also been highlighted in newspapers, magazines and radio programs.

- Ways to strengthen the societal impact of the RC's research and doctoral training.

In the long-term we can envisage that our basic research, discoveries, and inventions will benefit society and mankind by providing new hit and lead molecules. These, in turn, will be used for further development to achieve potent, efficient, safe and affordable drugs. In Europe and other parts of the world with high standard of living, diseases such as cancers are an increasing threat to public health. On the other hand, in developing countries, parasitic infectious diseases are an enormous health and economic challenge. Part of our research is focused on cancer (leukemias, prostate cancer) and tropical parasitic diseases (leishmaniasis). In the future, innovations based on our research could be available to combat these diseases. A concrete action to strengthen the RC's societal impact is developing our doctoral training to yield even higher quality PhDs for society. Another option is to develop collaboration between the RC and the drug industry, e.g. by attracting researchers from companies to the RC to learn new methods.



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### RC-SPECIFIC STAGE 2 MATERIAL

4 INTERNATIONAL AND NATIONAL (INCL. INTERSECTORAL) RESEARCH COLLABORATION AND RESEARCHER MOBILITY (MAX. 4400 CHARACTERS WITH SPACES)

- Description of the RC's research collaborations and joint doctoral training activities and how the RC has promoted researcher mobility.

The RC's doctoral students belong either to Graduate School in Pharmaceutical Research or National Doctoral Program in Informational and Structural Biology.

The RC's research collaboration may be described at local, domestic and international levels. The local collaborators are within our home university. The most important collaborators in the Faculty of Pharmacy are: Centre for Drug Research (bioactivity screening), Pharmaceutical Chemistry (analytical techniques), Pharmaceutical Technology (transport) and Pharmacology & Toxicology (protein kinases). The key collaborators in Viikki Campus are Institute of Biotechnology (alphaviruses, NMR, protein structures), Neuroscience Center (tyrosine kinases), Faculty of Veterinary Medicine (orexin), and Faculty of Agriculture (terpenes). The major collaborators in Meilahti Campus are from the Faculty of Medicine (kallikreins).

Other domestic collaborators are from the University of Eastern Finland (kallikreins), the Technical Research Centre of Finland (terpenes), the University of Tampere (inflammation), and from the Åbo Akademi (Chlamydia, structural bioinformatics).

Our closest Nordic collaborators are University of Gothenburg (kallikreins) and University of Copenhagen (synthesis methods). Other international collaborators are Universite de Lyon, University of Birmingham, University of Geneva & University of Milano-Bicocca (protein kinases); Hebrew University of Jerusalem & Universidad Complutense de Madrid (Leishmania); University of Ljubljana and KU Leuven (marine compounds); EFPL (Mycobacteria); Technische Universität Chemnitz (small molecule X-ray) and Martin-Luther-Universität Halle-Saale (modeling); Tufts University, USA, University of Arkansas for Medical Sciences, USA, and the Flinders Medical Centre, Australia (different aspects of UGTs research).

The RC is involved in the following FP6 or FP7 research projects of the EC: Protein Kinase Research, LIINTOP, FORESTSPECS, MAREX (see Ch. 2). The RC participates also the following COST networks: New drugs for neglected diseases & Combinatorial chemistry and the Paul Ehrlich MedChem Euro-PhD Network for doctoral training.

Another way in which the RC is involved in international collaborations is examination and evaluation of PhD theses. We almost always employ international opponent for the public examination of PhD theses of our students, often also send the theses for pre-examination by internationally-known scientists in the respective fields, and act ourselves as pre-examiners and opponents for PhD theses in other countries. We participate actively in international scientific meetings, symposia and seminars and present our research there.

How the RC has promoted researcher mobility?

Two doctoral students of the RC have carried out part of their research abroad, in the Universities of Gothenburg and Copenhagen. One RC student takes part in the Medicinal Chemistry Euro-PhD Network.

We have also attracted a number of international students and researchers at different levels, from undergraduate students for shorter periods (ERASMUS, COST) to those that do their postgraduate research in our laboratories, as well postdoctoral researchers.



## INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE UNIVERSITY OF HELSINKI

### RC-SPECIFIC STAGE 2 MATERIAL

- RC's strengths and challenges related to research collaboration and researcher mobility, and the actions planned for their development.

Strengths: RC is involved in excellent local [Viikki], domestic [Meilahti, Kumpula, VTT, Finnish universities and institutes], and in international networks (EU, COST, ERASMUS) and collaborations with high scientific/technological level. RC has gained strong management and organizational skills as coordinators of large international research consortia.

The evaluation panel of Chemistry Research in Finland (2005-9) stated of our RC: "The unit has much active collaboration within UH, as well as with other Finnish universities and institutes. Many industrial collaborations are effective through Tekes projects. The unit has succeeded in internationalisation, as evidenced by the presence of postdoctoral researchers and postgraduate students from abroad."

Challenges: Researcher mobility from RC to the foreign research institutes and universities could still be improved considerably. We hope that participation in EC-funded projects as well as the current COST and Euro-PhD programs would facilitate the international mobility from our RC.

#### 5 OPERATIONAL CONDITIONS (MAX. 4400 CHARACTERS WITH SPACES)

- Description of the operational conditions in the RC's research environment (e.g. research infrastructure, balance between research and teaching duties).

The RC has an experienced, qualified and motivated personnel, good instrumentation and external funding. Its scientists come from two administrative units of the Faculty: Division of Pharmaceutical Chemistry and Centre for Drug Research. The RC has infrastructure of both units at its disposal. The general technical and administrative infrastructure of UH is excellent (Helsinki University Library, Research Services, Information Technology, Personnel and Legal Services and Support for Teaching). However, the Finances of the University is unfortunately lacking behind as the tools provided for financial management of projects and research units are of mediocre quality. Moreover, its level of assistance and service has plenty of room for improvement.

Our biochemical, medicinal chemistry and synthesis laboratories are relatively well-equipped: 300 MHz Varian NMR spectrometer; Waters HPLC/MS instruments for both analytical and preparative work; Hewlett-Packard GC/MS (since 1988!); Bruker FTIR spectrometer equipped with an ATR device and a microscope; Biotage microwave synthesizer and parallel chromatography system; parallel solid-phase synthesizers for the hit/lead optimization. One of our RC groups has introduced DNA technologies and gene expression to the Faculty and maintains and uses the infrastructure to carry out gene cloning and expression as well as protein purification and analyses by state-of-the-art methods. For computational modeling started in 2008, a modern computer network and the necessary software obtained from academic licenses by the Finnish Center for Scientific Computing.

The RC has an access to many facilities in Viikki Campus via Instrument Centre, Core Facilities and other co-operation laboratories. Although there are many instruments available, some of them are very old and there is an urgent need for high-performance instruments for RC's research (a high-field NMR instrument and HPLC-MS for routine use).

Administrative duties: RC Members have had many positions of university and faculty administration: JYK: Head of the Division of the Pharmaceutical Chemistry; vice-dean in charge of research affairs; member: faculty council, board of Viikki Science Library, board of DDTC, planning committee, chemical management working group; chair of student selection committee; EW: member: committee for the academic affairs, student selection committee; vice-member: planning committee, advisory board of Viikki Campus Library; MF: member of the committee for research affairs. Finally, several RC researchers



## INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE UNIVERSITY OF HELSINKI

### RC-SPECIFIC STAGE 2 MATERIAL

were appointed as members of various permanent and ad hoc committees of the Faculty during 2005-10.

Educational duties: Our RC is responsible for BSc, MSc and PhD level lecture and practical courses (54 cu) in the Faculty (medicinal, pharmaceutical and organic chemistry; drug metabolism, computer-aided drug discovery; molecular and cell biology, biochemistry). The RC members supervise a relatively large number of under and postgraduate studies and are also involved in the supervision of postgraduate studies in other units of UH and domestic universities. The RC also provides the undergraduates of Faculty of Biosciences and Helsinki Region Biotechnology Educational Program with extensive organic chemistry course package (9 cu).

- RC's strengths and challenges related to operational conditions, and the actions planned for their development.

Strengths: The RC has good infrastructure with relatively modern instrumentation. Our RC has an experienced, qualified and dedicated personnel and good external funding.

Challenges: Mechanisms of purchasing expensive research instruments and equipment in a coordinated and fair manner as well as of financing instrument repairs both in the Faculty and University level are insufficient. The most urgent research instruments needed are the new high-field NMR spectrometer and a robust routine HPLC-MS for the routine use of RC. In addition, lack of personnel responsible for instrument maintenance, routine laboratory operations and computational infrastructure support increases the workload of the RC members. Computational modelling would greatly benefit from an on-site IT specialist, available in other Finnish universities, such as UEF and AA.

Finally one of our major endemic/generic challenges is the continuously increasing workload in terms of faculty and university bureaucracy and related administration, which seriously depletes human resources for research and doctoral training.

#### 6 LEADERSHIP AND MANAGEMENT IN THE RESEARCHER COMMUNITY (MAX. 4400 CHARACTERS WITH SPACES)

- Description of the execution and processes of leadership in the RC, how the management-related responsibilities and roles are distributed in the RC and how the leadership- and management-related processes support high quality research, collaboration between principal investigators and other researchers in the RC, the RC's research focus and strengthening of the RC's know-how.

The RC combines the complementary expertise of two units of the Faculty: Division of Pharmaceutical Chemistry (DPC) and Centre for Drug Research (CDR). Principal investigators Erik Wallén and Jari Yli-Kauhaluoma are from the Medicinal Chemistry research group of the DPC. Principal investigators Henri Xhaard and Moshe Finel represent CDR and its Computational Drug Discovery group and the Molecular and Biochemical Pharmacology group. The four principal investigators are responsible for research strategy of the RC, implementation of the objectives of their research projects and the respective plans of actions. The major principles of RC leadership are appreciation, interaction and trust at all levels. These help us to create an open and innovative research environment and an excellent working spirit as well as to encourage our doctoral students to present their own ideas.

In general RC adheres to the Strategic Plan for the University and in particular to the research strategies of DPC and CDR. The main strategic objective is to maintain high standards and a high profile of the RC research and its further development in the long term. As a tool of research management we use regular self-assessments and "benchmarking" by monitoring our key figures of scientific productivity and quality and comparing them against those of an internationally established research unit, the



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Leiden/Amsterdam Center for Drug Research. We feel that self-assessments like this help us to maintain high standards and a high profile of research. In fact, the report of an International Evaluation of Chemistry Research in Finland 2005-9 by the Academy of Finland concluded of our RC that "The unit should maintain its research direction and level of achievement, which is of high quality in an important societal area."

Our RC attempts to establish a clear connection between strategic objectives of the University, DPC & CDR and various operative level practises especially by regular discussions about the strategic aims with the members of RC and divisions of the Faculty. For example, all the RC research teams have regular bi- or triweekly group meetings for the discussions dealing with progress of research and related administrative issues. The respective administrative units (DPC, CDR) have their own meetings for the discussions about the research strategies of the units. Moreover, the Lammi Research Seminar of the Faculty, organized annually since 2001, has become a natural forum for discussions about science, research, doctoral training and research strategies of the research groups and Faculty.

The strengthening of know-how of the RC members takes place first and foremost via our research projects and participation to the domestic and international research programmes and networks. The RC researchers attend regularly domestic and international scientific meetings, conferences, seminars and symposia. Our RC openly supports these activities.

Finally we actively support the diversity in our RC. Despite there being no female PIs in our RC, 32% (n=11) from the scientists contributing to the RC are females, at different stages of their careers, and at different stages of their private and family life. The proportion of foreign scholars and students is 38% (n=13) in our RC.

- RC's strengths and challenges related to leadership and management, and the actions planned for developing the processes.

Our strengths are in a successful maintenance of research direction and level of achievement. Thanks to experienced, qualified and dedicated personnel we have maintained excellent working spirit and kept research aims clear. Our research projects also form a synergistic entity.

Challenges relate to the fact that RC teams belong to two separate administrative units. Despite clear scientific foci of RC teams, creation of a unified and coherent research strategy for the RC may be hampered as a whole. Teaching obligations of the units also differ significantly from each other. The CDR members use a maximum 5% of the annual 1600-h workload for teaching, while the corresponding figures in DPC range from 5 to as high as 30%.

Finally we feel that continuously increasing workload in the faculty and university bureaucracy, administration and other secondary actions depletes resources of research and doctoral training. A concrete challenge is to prioritize the administrative actions and execute only the most important ones, i.e. those that promote high quality research and doctoral training.

#### 7 EXTERNAL COMPETITIVE FUNDING OF THE RC

- Listing of the RCs external competitive funding, where:
  - the funding decisions have been made during 1.1.2005-31.12.2010, and
  - the administrator of the funding is/has been the University of Helsinki
- Academy of Finland (AF) - total amount of funding (in euros) AF has decided to allocate to the RC members during 1.1.2005-31.12.2010: 1110000



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- Finnish Funding Agency for Technology and Innovation (TEKES) - total amount of funding (in euros) TEKES has decided to allocate to the RC members during 1.1.2005-31.12.2010: 670000
- European Union (EU) - total amount of funding (in euros) EU has decided to allocate to the RC members during 1.1.2005-31.12.2010: 1580000
- European Research Council (ERC) - total amount of funding (in euros) ERC has decided to allocate to the RC members during 1.1.2005-31.12.2010: 0
- International and national foundations – names of international and national foundations which have decided to allocate funding to the RC members during 1.1.2005-31.12.2010, and the amount of their funding (in euros).
  - names of the foundations: Sigrid Juselius Foundation (268500 eur), Center for International Mobility (34480 eur), Walter och Lisi Wahls stiftelse för naturvetenskaplig forskning (10000 eur), Research Foundation for Clinical Chemistry (10000 eur), Päivikki & Sakari Sohlberg Foundation (70000 eur), Foundation for Research of Natural Resources in Finland (122000 eur), Marjatta ja Eino Kollin Säätiö (180000 eur), University of Helsinki research foundation (22000 eur)
  - total amount of funding (in euros) from the above-mentioned foundations: 720000
- Other international funding - names of other international funding organizations which have decided to allocate funding to the RC members during 1.1.2005-31.12.2010, and the amount of their funding (in euros).
  - names of the funding organizations: World Anti-Doping Agency, WADA (61000 eur, 166500 eur, 81600 eur)
  - total amount of funding (in euros) from the above-mentioned funding organizations: 310000
- Other national funding (incl. EVO funding and Ministry of Education and Culture funded doctoral programme positions) - names of other national funding organizations which have decided to allocate funding to the RC members during 1.1.2005-31.12.2010, and the amount of their funding (in euros).
  - names of the funding organizations: Forestcluster Ltd. (160000 eur), Biocenter Finland (28000 eur), Ministry of Education and Culture (310000 eur)
  - total amount of funding (in euros) from the above-mentioned funding organizations: 500000

8 RC'S STRATEGIC ACTION PLAN FOR 2011–2013 (MAX. 4400 CHARACTERS WITH SPACES)

- Description of the RC's future perspectives in respect to research and doctoral training.

The cornerstone of our research strategy is excellent research and educational results that have been achieved in the research areas, where we are already at international high level or soon approaching it (please see Chapter 1). During 2011-2013 our RC will focus to medicinal chemistry and biochemistry research of the following themes: (i) medicinal chemistry of cancer chemotherapy (protein kinase research and peptidomimetics of kallikreins), (ii) new antibiotics and antivirals against intracellular pathogens (*Leishmania* sp., *Chlamydia pneumoniae*, Alphavirus), (iii) metabolism of drugs and other xenobiotics and (iv) medicinal chemistry of G protein-coupled receptors (orexin, alpha-2 adrenergic receptors). We intend to strengthen these research areas, integrate them better with each other, and pay careful attention to the selection of possible new research areas to. New research areas for our RC



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are expected to support the existing work or they should be so revolutionary in nature so that we will focus all our efforts to them, if we are convinced that they are groundbreaking areas.

One of our aims is to increase research with considerable risk that is based on original basic research of our RC. We hope to have the means to support long-term basic, original and high quality research, as we believe that it only is capable of yielding the best results in the future. Our aim is also (i) to continue doing multidisciplinary research by recruiting scientists with various and complementary backgrounds in the fields such as chemistry, pharmaceutical sciences, biology and biochemistry, (ii) to continue working with our current collaborators, (iii) to continue finding new domestic and international collaborators, who can help us to reach the highest international level in our selected research areas, and (iv) to continue publishing our research results in high quality journals of the field.

There are several actions which we will do to support these strategic aims. We will place more emphasis on recruiting new and suitable staff. We will aim at (i) employing more post-doctoral researchers in our RC, (ii) supporting academic careers of young promising researchers, (iii) continuing and increasing high-quality domestic and international collaborations, and (iv) investing in education of postgraduate and undergraduate students. We are planning to recruit the best undergraduate students by continuing to provide them with a possibility to join our multidisciplinary research groups already at early stages of their studies in the Faculty of Pharmacy. In addition, improvement of research infrastructure is an important supporting action. Currently, there is a need for improved instrumentation (e.g. a high-field NMR instrument and a robust HPLC-MS).

We promote advancement of science by encouraging our researchers to present their own ideas, promoting co-operation with national and international research groups, supporting international researcher exchange, and most importantly participating actively in European and global research networks. The co-operation with industry and private laboratories is an essential part of the implementation of the research aims for the benefit of society and mankind.

The well-being of our personnel is taken care by open management policy and by maintaining innovative and co-operative working atmosphere in our RC. It is also important to be visible in scientific meetings and organizations, for example by organizing international researcher meetings, courses, seminars, workshops etc., as well as in society in general to point out the significance of medicinal chemistry and biochemistry in the drug discovery and development process and to be able to make an effort to ensure long-term funding to support basic research, recruitment of the best scientists and improvement of infrastructure. We will also take an active role in popularizing our research to the larger audience.

9 SHORT DESCRIPTION OF HOW THE RC MEMBERS HAVE CONTRIBUTED TO THE COMPILATION OF THE STAGE 2 MATERIALS (MAX. 1100 CHARACTERS WITH SPACES).

After the preparatory discussions and planning meeting of the MedChemBio RC evaluation, JYK prepared the first draft of the stage 2 materials and sent it to other principal investigators of the RC (EW, MF, HX) for comments and further writing and editing. The resulting 2nd draft was circulated for additional changes, comments and proofreading. The final third version of the stage 2 material was accepted as a final submission version of the evaluation package.





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**1 Analysis of publications**

- Associated person is one of Moshe Finel , Erik Wallen , Henri Xhaard , Jari Yli-Kauhaluoma  
, Ingo Aumuller , Kirsi Harju , Paula Kiuru ,  
, Liisa Laakkonen , Mohanathas Rajaratnam , Leslie Regad ,  
, Swapan Kumar Samanta, Andrew Charles Tadd , Sami Aleksi Alakurtti , Martti Alkio ,  
, Ingo Bichlmaier , Gustav Boije af Gennäs , Raissa Haavikko  
, Sanna Kaivosääri , Leena Keurulainen , Alexandros Kiriazis ,  
, Mika Kurkela , Tuomo Kaarlo Erik Leikoski , Nenad Manevski ,  
, Kristian Meinander , Antti Siiskonen , Nina Sneitz ,  
Taina Sten , Michal Andzej Stepniewski , Mikko Vahermo , Gloria Wissel ,  
Hongbo Zhang , Yuezhou Zhang ,

Publication type	Publication year						Total Count 2005 - 2010
	2005	2006	2007	2008	2009	2010	
A1 Refereed journal article	20	18	21	21	21	22	123
A2 Review in scientific journal	2	1		1			4
A4 Article in conference publication (refereed)	2			2	3	1	8
B1 Unrefereed journal article		1	1				2
B3 Unrefereed article in conference proceedings	1						1
C2 Edited book, compilation, conference proceeding or special issue of journal			1				1
D2 Article in professional hand or guide book or in a professional data system, or text book material				1			1
H1 Patents						2	2



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**2 Listing of publications**

**A1 Refereed journal article**

**2005**

- Alonen, A, Aitio, O, Hakala, K, Luukkanen, L, Finel, M, Kostiaainen, R **2005**, 'Biosynthesis of dobutamine monoglucuronides and glucuronidation of dobutamine by recombinant human UDP-glucuronosyltransferases', **Drug Metabolism and Disposition**, vol 33, no. 5, pp. 657-663.
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- Jarho, E, Wallen, EAA, Christiaans, J, Forsberg, M, Venäläinen, J, Männistö, PT, Gynther, J, Poso, A **2005**, 'Dicarboxylic acid azacycle L-prolyl-pyrrolidine amides as prolyl oligopeptidase inhibitors and three-dimensional quantitative structure-activity relationship of the enzyme-inhibitor interactions', **Journal of Medicinal Chemistry**, vol 48, no. 15, pp. 4772-4782.
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- Kärkkäinen, J, Forsström, T, Tornaeus, J, Wähälä, K, Kiuru, P, Honkanen, A, Stenman, U, Turpeinen, U, Hesso, A **2005**, 'Potentially hallucinogenic 5-hydroxytryptamine receptor ligands bufotenine and dimethyltryptamine in blood and tissues', **Scandinavian Journal of Clinical & Laboratory Investigation**, vol 65, no. 3, pp. 189-199.
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- Samanta, S, Yli-Kauhaluoma, J **2005**, 'Polymer-supported 1,3-Oxazolium-5-olates: synthesis of 1,2,4-Triazoles', **Journal of Combinatorial Chemistry**, vol 7, no. 1, pp. 142-146.
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Vahermo, M, Leinonen, A, Suominen, T, Kolmonen, M, Kuuranne, T, Yli-Kauhaluoma, J **2009**, 'Synthesis of 17-Dihydroexemestane as a Reference Compound in Doping Control', in **Proceedings of the Manfred Donike Workshop**, pp. 327-330 **Recent advances in doping analysis, no. 17**.

**2010**

Mirza, S, Miroshnyk, I, Mohammadi, G, Alakurtti, SA, Hussain, M, Yli-Kauhaluoma, J, Urtti, A **2010**, *Electrospinning platform for fabrication of monodispersed nanoparticles for pharmaceutical applications.*, Paper presented at **2010 FIP Pharmaceutical Sciences World Congress, New Orleans**, United States. 14. - 18. November, 2010. AAPS Journal 12 S2 SPRINGER NEW YORK LLC.

**B1 Unrefereed journal article**

**2006**

Yli-Kauhaluoma, J, Sivonen, K, Tuominen, RK **2006**, 'Protein kinase research in the University of Helsinki', **Dosis**, vol 22, no. 2, pp. 152-7.

**2007**

Lemberg, K, Korpi, E, Siiskonen, A, Yli-Kauhaluoma, J, Kontinen, VK, Viljakka, K, Kalso, E, Korpi, ER **2007**, 'Oxycodone's mechanism of action and potency differences after spinal and systemic routes of administration: [reply]', **Anesthesiology**, vol 106, no. 5, pp. 1064-1065.

**B3 Unrefereed article in conference proceedings**

**2005**





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UNIVERSITY OF HELSINKI

RC-SPECIFIC TUHAT COMPILATIONS OF PUBLICATIONS DATA 2005-2010

MEDCHEMBIO/Yli-Kauhaluoma

Wähälä, K, Kiuru, P, Leppälä, E, Pohjoispää, M, Parikka, K, Raffaelli, B **2005**, *Controlled Polydeuteration of Estrogenic Compounds*, Paper presented at **Workshop of the Central European Division e.V. of the International Isotope Society, Bad Soden, Germany**, 16. - 17. June, 2005. *Journal of Labelled Compounds & Radiopharmaceuticals* 49 JOHN/WILEY & SONS LTD..

**C2 Edited book, compilation, conference proceeding or special issue of journal**

**2007**

Yli-Kauhaluoma, J (ed.) **2007**, *The Taskinen Symposium on Drug Design and Metabolism: Faculty of Pharmacy, University of Helsinki August 17.18, 2007*, Helsingin yliopisto, farmasian tiedekunta, Helsinki.

**D2 Article in professional hand or guide book or in a professional data system, or text book material**

**2008**

Aumüller, I, Yli-Kauhaluoma, J **2008**, 'The preferred conformations of heptafulvenes are determined by various factors', in A Sillanpää et al. (ed.), *CSC report on computational science in Finland 2006-2007*, CSC - Scientific Computing Ltd., Espoo, pp. 89-93.

**H1 Patents**

**2010**

Yli-Kauhaluoma, J, Koskimies, S, Alakurtti, SA, Bergström, P, Mäkelä, T, Vuorela, P, Tammela, P, Minkkinen, J, Pohjala, L Nov. 30 2010, *Betuliiniperäiset yhdisteet antimikrobisina aineina*, 121468.

Yli-Kauhaluoma, J, Pitkänen, P, Heiskanen, N, Wähälä, K, Hulkko, J, Koskimies, S Jan. 29 2010, *Menetelmä oligo-/polyestereiden valmistamiseksi suberiinin ja/tai kutiinidin karboksyylihapposeoksesta*, FI-120684.



INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE  
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RC-SPECIFIC TUHAT COMPILATIONS OF OTHER SCIENTIFIC ACTIVITIES 2005-2010

MEDCHEMBIO/Yli-Kauhaluoma

**1 Analysis of activities 2005-2010**

- Associated person is one of Moshe Finel , Erik Wallen , Henri Xhaard , Jari Yli-Kauhaluoma  
, Ingo Aumuller , Kirsi Harju , Paula Kiuru ,  
, Liisa Laakkonen , Mohanathas Rajaratnam , Leslie Regad ,  
, Swapan Kumar Samanta, Andrew Charles Tadd , Sami Aleksi Alakurtti , Martti Alkio ,  
, Ingo Bichlmaier , Gustav Boije af Gennäs , Raisa Haavikko  
, Sanna Kaivosääri , Tuomo Kaarlo Erik Leikoski , Leena Keurulainen , Alexandros Kiriazis ,  
, Mika Kurkela , Antti Siiskonen , Nenad Manevski ,  
, Kristian Meinander , Mikko Vahermo , Nina Sneitz ,  
Taina Sten , Michal Andzej Stepniewski , Gloria Wissel ,  
Hongbo Zhang , Yuezhou Zhang ,

Activity type	Count
Supervisor or co-supervisor of doctoral thesis	33
Prizes and awards	3
Editor of research journal	1
Peer review of manuscripts	28
Editor of special theme number	1
Assessment of candidates for academic posts	3
Membership or other role in review committee	12
Membership or other role in research network	7
Membership or other role in national/international committee, council, board	19
Membership or other role in public Finnish or international organization	4
Participation in interview for written media	9
Participation in TV programme	1



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RC-SPECIFIC TUHAT COMPILATIONS OF OTHER SCIENTIFIC ACTIVITIES 2005-2010

MEDCHEMBIO/Yli-Kauhaluoma

## 2 Listing of activities 2005-2010

### Supervisor or co-supervisor of doctoral thesis

#### **Moshe Finel ,**

Co-supervisor of Ph.D. research, Moshe Finel, 2000 → 2006, Finland  
Co-supervisor of PhD research, Moshe Finel, 2004 → 2009, Finland  
Co-supervisor of Ph.D. research, Moshe Finel, 2005 → 2008  
Co-supervisor of Ph.D. research, Moshe Finel, 2005 → 2007  
Supervisor of Ph.D. research, Moshe Finel, 2005 → 2010  
Supervisor of Ph.D. research, Moshe Finel, 2005 → 2010  
Co-supervisor of Ph.D. research, Moshe Finel, 2006 → 2009  
Supervisor of Ph.D. research, Moshe Finel, 2007 → 2011

#### **Erik Wallen ,**

Main supervisor of doctoral thesis of Elina M. Jarho, completed in Feb. 2007, Erik Wallen, 2000 → 2007, Finland  
Main supervisor of doctoral thesis of Päivi H. Kiviranta, completed in Dec. 2008, Erik Wallen, 2003 → 2008, Finland  
Main supervisor of doctoral thesis of Kristian Meinander, not yet completed, Erik Wallen, 2007 → ..., Finland

#### **Henri Xhaard ,**

Co-supervision of Doctoral thesis, Henri Xhaard, 2009 → ...  
Co-supervision of Doctoral thesis, Henri Xhaard, 2010 → ...  
Supervision of Doctoral thesis, Henri Xhaard, 2010 → ...  
Supervision of Doctoral thesis, Henri Xhaard, 2010 → ...  
Supervision of doctoral thesis, Henri Xhaard, 2010 → ...

#### **Jari Yli-Kauhaluoma ,**

Supervisor: Carbon-carbon Bond Formation on Solid Phase, Jari Yli-Kauhaluoma, 01.03.2000 → ..., Finland  
Supervisor: Dependence of Enzymatic Glucuronidation of Phenolic Compounds on Their  $pK_a$  Values: A Basic Approach for the Design of Inhibitors for the UDP-Glucuronosyltransferase Isoenzyme UGT1A9, Jari Yli-Kauhaluoma, 2002 → 2005, Germany  
Supervisor: Polymer-supported Diels-Alder Reactions and Pim Kinases, Jari Yli-Kauhaluoma, 01.06.2002 → ..., Finland  
Supervisor: Synthesis of 1,2,3-Triazoles by the Reaction Between Azides and Enamines, Jari Yli-Kauhaluoma, 2003 → 2007, Finland  
Supervisor: Design and Synthesis of Protein Kinase C and Anaplastic Lymphoma Kinase Inhibitors, Jari Yli-Kauhaluoma, 01.03.2004 → ..., Finland  
Supervisor: Medicinal Chemistry of Birch Triterpenes, Jari Yli-Kauhaluoma, 08.03.2004 → ..., Finland  
Supervisor: Microchip-Based Combinatorial Chemistry, Jari Yli-Kauhaluoma, 01.08.2004 → ..., Finland  
Supervisor: Synthesis of Metabolites of Psychostimulants, Anticestrogens, Aromatase Inhibitors and  $\beta$ -blockers, Jari Yli-Kauhaluoma, 01.01.2004 → ..., Finland  
Supervisor: Design and Synthesis of Compounds against *Chlamydia pneumoniae*, Jari Yli-Kauhaluoma, 01.01.2006 → ..., Finland  
Supervisor: Selective Inhibitors of the Human UDP-glucuronosyltransferases, Jari Yli-Kauhaluoma, 01.11.2007 → ..., Finland  
Supervisor: Antibiotics against *Chlamydia pneumoniae*, Jari Yli-Kauhaluoma, 01.03.2008 → ..., Finland  
Supervisor: Purification of Pharmaceuticals and Nutraceutical Compounds by Sub- and Supercritical Chromatography and Extraction, Jari Yli-Kauhaluoma, 08.02.2008, Finland  
Supervisor: Stereochemical and Steric Control of Enzymatic Glucuronidation. A Rational Approach for the Design of Novel Inhibitors for the Human UDP-Glucuronosyltransferase 2B7, Jari Yli-Kauhaluoma, 22.02.2008, Finland



INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE  
UNIVERSITY OF HELSINKI

RC-SPECIFIC TUHAT COMPILATIONS OF OTHER SCIENTIFIC ACTIVITIES 2005-2010

MEDCHEMBIO/Yli-Kauhaluoma

Supervisor: Synthesis of Nitrogen-Containing, Five-Membered Heterocycles. 1,3-Dipolar Cycloadditions, Solid-Phase Techniques, and Parallel Methods, Jari Yli-Kauhaluoma, 30.10.2009, Finland

Supervisor: Terpene Syntheses, Jari Yli-Kauhaluoma, 01.05.2009 → ..., Finland

Supervisor: Triterpene Derivatives against Trypanosomatidae, Jari Yli-Kauhaluoma, 01.03.2010 → ..., Finland

**Paula Kiuru ,**

Supervisor: Antibiotics against Chlamydia pneumoniae, Paula Kiuru, 01.03.2008 → ..., Finland

**Prizes and awards**

**Kirsi Harju ,**

Best PhD thesis of the Graduate School in Pharmaceutical Research 2009, Kirsi Harju, 2010, Finland

**Ingo Bichmaier ,**

Best PhD Thesis of the Graduate School in Pharmaceutical Research 2009, Ingo Bichmaier, 2009, Finland

Albert Wuokko Award 2010, Ingo Bichmaier, 2010

**Editor of research journal**

**Jari Yli-Kauhaluoma ,**

Anti-Cancer Agents in Medicinal Chemistry, Jari Yli-Kauhaluoma, 01.01.2009 → ..., United States

**Peer review of manuscripts**

**Moshe Finel ,**

Peer review of many manuscripts, an ongoing activity, Moshe Finel, 01.01.1996 → ...

**Erik Wallen ,**

Regular peer review of manuscripts, Erik Wallen, 2003 → ...

**Jari Yli-Kauhaluoma ,**

Peer reviewer: Journal of Chemical Education, Jari Yli-Kauhaluoma, 30.11.2003 → ..., United States

Peer reviewer: Chemical Communications, Jari Yli-Kauhaluoma, 14.07.2004 → ..., United Kingdom

Peer reviewer: Chemical Society Reviews, Jari Yli-Kauhaluoma, 06.09.2004 → ..., United Kingdom

Peer reviewer: Green Chemistry, Jari Yli-Kauhaluoma, 06.01.2004 → ..., United Kingdom

Peer reviewer: Journal of Combinatorial Chemistry, Jari Yli-Kauhaluoma, 02.02.2004 → ..., United States

Peer reviewer: Organic & Biomolecular Chemistry, Jari Yli-Kauhaluoma, 10.02.2004 → ..., United Kingdom

Peer reviewer: The Journal of Organic Chemistry, Jari Yli-Kauhaluoma, 08.07.2004 → ..., United States

Peer reviewer: Bioorganic & Medicinal Chemistry Letters, Jari Yli-Kauhaluoma, 21.12.2005 → ..., United States

Peer reviewer: Molecular BioSystems, Jari Yli-Kauhaluoma, 08.09.2005, United Kingdom

Peer reviewer: Tetrahedron, Jari Yli-Kauhaluoma, 13.04.2005 → ..., United States

Peer reviewer: Chirality, Jari Yli-Kauhaluoma, 06.07.2006, United States

Peer reviewer: European Journal of Medicinal Chemistry, Jari Yli-Kauhaluoma, 07.11.2006, Netherlands

Peer reviewer: European Journal of Pharmaceutical Sciences, Jari Yli-Kauhaluoma, 14.09.2006 → ..., Finland

Peer reviewer: Journal of Medicinal Chemistry, Jari Yli-Kauhaluoma, 09.02.2006 → ..., United States

Peer reviewer: Molecules, Jari Yli-Kauhaluoma, 13.01.2008, Switzerland

Peer reviewer: Tetrahedron Letters, Jari Yli-Kauhaluoma, 16.06.2008 → ..., United States

Peer reviewer: Acta Chimica Slovenica, Jari Yli-Kauhaluoma, 29.12.2009, Slovenia

Peer reviewer: Bioorganic & Medicinal Chemistry, Jari Yli-Kauhaluoma, 01.01.2009 → ..., United States

Peer reviewer: Proceedings of the National Academy of Sciences USA, Jari Yli-Kauhaluoma, 16.12.2009 → ..., United States



## INTERNATIONAL EVALUATION OF RESEARCH AND DOCTORAL TRAINING AT THE UNIVERSITY OF HELSINKI

### RC-SPECIFIC TUHAT COMPILATIONS OF OTHER SCIENTIFIC ACTIVITIES 2005-2010

#### MEDCHEMBIO/Yli-Kauhaluoma

Peer reviewer: Anti-Cancer Agents in Medicinal Chemistry, Jari Yli-Kauhaluoma, 17.01.2010 → ..., United States

Peer reviewer: British Journal of Pharmacology, Jari Yli-Kauhaluoma, 01.06.2010, United Kingdom

Peer reviewer: Current Topics in Medicinal Chemistry, Jari Yli-Kauhaluoma, 01.03.2010 → ..., United States

Peer reviewer: Journal of the Serbian Chemical Society, Jari Yli-Kauhaluoma, 15.11.2010, Serbia

Peer reviewer: Synlett, Jari Yli-Kauhaluoma, 02.08.2010, Germany

#### **Paula Kiuru ,**

Current Topics in Medicinal Chemistry, Paula Kiuru, 01.2010

Organic & Biomolecular Chemistry, Paula Kiuru, 10.2010

#### **Editor of special theme number**

##### **Jari Yli-Kauhaluoma ,**

Guest Editor: Current Topics in Medicinal Chemistry, Jari Yli-Kauhaluoma, 2009 → 2011, United States

#### **Assessment of candidates for academic posts**

##### **Jari Yli-Kauhaluoma ,**

Associate Professorship in Chemistry, National University of Singapore, Singapore, Jari Yli-Kauhaluoma, 2006, Singapore

Chair of the professorship evaluation board, Jari Yli-Kauhaluoma, 2009, Finland

The Lead Research Fellow in Bioorganic Chemistry, University of Tartu, Estonia, Jari Yli-Kauhaluoma, 06.05.2010 → 14.05.2010, Estonia

#### **Membership or other role in review committee**

##### **Erik Wallen ,**

Evaluation of funding applications, Erik Wallen, 2008 → ..., Belgium

Evaluation of grant applications, Erik Wallen, 2010 → ..., Finland

##### **Jari Yli-Kauhaluoma ,**

Reviewer of research grant applications (INTAS), Jari Yli-Kauhaluoma, 2003 → 2006, Belgium

Reviewer of research grant applications (ETF), Jari Yli-Kauhaluoma, 2004 → 2006, Estonia

Reviewer for the positions of postdoctoral researchers (UHEL), Jari Yli-Kauhaluoma, 2006, Finland

Reviewer of research grant application (NSF), Jari Yli-Kauhaluoma, 2006 → 2007, United States

Reviewer of research grant applications (MATINE), Jari Yli-Kauhaluoma, 2006 → 2013, Finland

Reviewer of research grant applications (A\*STAR), Jari Yli-Kauhaluoma, 2007, Singapore

Reviewer of research grant applications, Jari Yli-Kauhaluoma, 21.12.2009 → 20.01.2010, Denmark

Reviewer of research grant applications (GACR), Jari Yli-Kauhaluoma, 2009, Czech Republic

Reviewer of research grant applications, Jari Yli-Kauhaluoma, 30.09.2010 → 20.10.2010, Serbia

##### **Paula Kiuru ,**

Reviewer of research grant applications, Paula Kiuru, 2005, Czech Republic

#### **Membership or other role in research network**

##### **Jari Yli-Kauhaluoma ,**

Head of the Design and Synthesis Group, Viikki Drug Discovery Technology Center (DDTC), Jari Yli-Kauhaluoma, 01.09.2000 → 30.06.2005, Finland

Viikki Research Groups in Biosciences, Jari Yli-Kauhaluoma, 01.09.2000 → ..., Finland

Member of the Project Coordination Committee of the FP6 Project: Protein Kinases - Novel Drug Targets for Post Genomic Era (LSHB-CT-2004-503467), Jari Yli-Kauhaluoma, 01.03.2004 → 31.08.2009, Finland

Member of the Management Committee of the COST Programme CM0801, Jari Yli-Kauhaluoma, 18.06.2008 → 27.11.2012, Finland



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#### MEDCHEMBIO/Yli-Kauhaluoma

Vice co-ordinator of the FP7 project FORESTSPECS, Jari Yli-Kauhaluoma, 01.05.2009 → 30.04.2012, Finland

Member of the Board of the Paul Ehrlich MedChem Euro-PhD Network, Jari Yli-Kauhaluoma, 01.01.2010 → 31.12.2013, Finland

Vice co-ordinator of the FP7 project MAREX, Jari Yli-Kauhaluoma, 01.08.2010 → 31.07.2014, Finland

#### **Membership or other role in national/international committee, council, board**

##### **Erik Wallen ,**

Executive committee member of the Finnish Pharmaceutical Society, Erik Wallen, 2009 → ..., Finland

Finnish delegate in the council of the European Federation for Medicinal Chemistry (EFMC), Erik Wallen, 2010 → ...

##### **Jari Yli-Kauhaluoma ,**

Member of the American Chemical Society, Jari Yli-Kauhaluoma, 1992 → ..., United States

Member of the Sigma Xi, The Scientific Research Society, Jari Yli-Kauhaluoma, 1998 → ..., United States

Member of the management group of the Viikki Drug Discovery Technology Center (DDTC), Jari Yli-Kauhaluoma, 01.09.2000 → 30.06.2005, Finland

Co-ordinator of the Drug Discovery Research Programme of the Biocenter Viikki Research Group Organization, Jari Yli-Kauhaluoma, 01.01.2001 → 31.12.2008, Finland

Deputy Member of the Faculty Council, Faculty of Pharmacy, University of Helsinki, Jari Yli-Kauhaluoma, 01.01.2004 → 31.12.2009, Finland

Deputy Member of the Research Committee, Faculty of Pharmacy, University of Helsinki, Jari Yli-Kauhaluoma, 01.01.2004 → 31.12.2009, Finland

Member of the Board of the Drug Discovery Technology Center (DDTC) of the University of Helsinki, Jari Yli-Kauhaluoma, 01.01.2005 → 31.12.2005, Finland

Member of the Chemical Committee of the University of Helsinki, Jari Yli-Kauhaluoma, 2005 → 2010, Finland

CBRN Division of the Scientific Advisory Board for Defence (MATINE), Jari Yli-Kauhaluoma, 17.05.2006 → 31.12.2013, Finland

Chair of the Admissions Committee, Faculty of Pharmacy, University of Helsinki, Jari Yli-Kauhaluoma, 01.01.2007 → 31.12.2009, Finland

Member of the Board of the Viikki Science Library of the University of Helsinki, Jari Yli-Kauhaluoma, 01.01.2007 → 31.12.2009, Finland

Pharmacopoeia Committee of the National Agency of Medicines, Jari Yli-Kauhaluoma, 01.03.2008 → 26.10.2009, Finland

Member of the Board: Paul Ehrlich European Medicinal Chemistry Ph.D. Network (Euro-PhD), Jari Yli-Kauhaluoma, 01.08.2009 → ..., Finland

Chair of the Research Committee, Faculty of Pharmacy, University of Helsinki, Jari Yli-Kauhaluoma, 01.01.2010 → 31.07.2010, Finland

Member of the Faculty Council, Faculty of Pharmacy, University of Helsinki, Jari Yli-Kauhaluoma, 01.01.2010 → 31.12.2013

Member of the Steering Group of the ChemistryLab Gadolin, Jari Yli-Kauhaluoma, 2010 → ..., Finland

Pharmacopoeia Committee of the Finnish Medicines Agency, Jari Yli-Kauhaluoma, 01.01.2010 → 28.02.2013, Finland

#### **Membership or other role in public Finnish or international organization**

##### **Jari Yli-Kauhaluoma ,**

Chief research scientist: Technical Research Centre of Finland (VTT), Jari Yli-Kauhaluoma, 01.01.2001 → ..., Finland

Vice-dean of the Faculty of Pharmacy in charge of research and doctoral training, Jari Yli-Kauhaluoma, 01.01.2010 → 31.07.2010, Finland

Vice-director of the Graduate School in Pharmaceutical Research, Jari Yli-Kauhaluoma, 01.01.2010 → 31.12.2011, Finland

##### **Paula Kiuru ,**

Board member, Paula Kiuru, 2010 → ..., Finland

#### **Participation in interview for written media**

##### **Jari Yli-Kauhaluoma ,**

Mediautiset-lehti, Jari Yli-Kauhaluoma, 07.10.2005 → 31.12.2011, Finland



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RC-SPECIFIC TUHAT COMPILATIONS OF OTHER SCIENTIFIC ACTIVITIES 2005-2010

MEDCHEMBIO/Yli-Kauhaluoma

Tuohesta voi tulla lääke, Jari Yli-Kauhaluoma, 07.10.2005, Finland

Työvoimatilanne ja proviisoripiskelijöiden sisäänottomäärät: Mikä on oikea tasapaino?, Jari Yli-Kauhaluoma, 2007 → ..., Finland

Kemiaa mitalin kääntöpuolelta, Jari Yli-Kauhaluoma, 22.08.2008, Finland

Healing waste from a pulp mill, Jari Yli-Kauhaluoma, 2009, Finland

Lääkekemia imaisi pikku kemistin, Jari Yli-Kauhaluoma, 28.08.2009, Finland

Tonneittain tuolta, Jari Yli-Kauhaluoma, 18.06.2009, Finland

Apteekkikokemusta metsästämissä, Jari Yli-Kauhaluoma, 2010, Finland

Metyleenidioksiapyrovaleroni, Jari Yli-Kauhaluoma, 2010, Finland

**Participation in TV programme**

**Jari Yli-Kauhaluoma ,**

Koivunkuoresta apua alkueläintauteihin?, Jari Yli-Kauhaluoma, 01.07.2009, Finland



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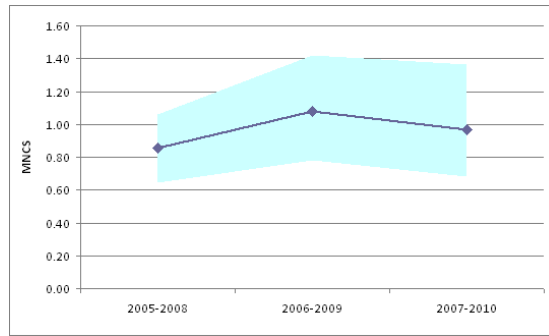
Web of Science(WoS)-based bibliometrics of the RC's publications data 1.1.2005-31.12.2010  
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Research Group: Yli-Kauhaluoma J

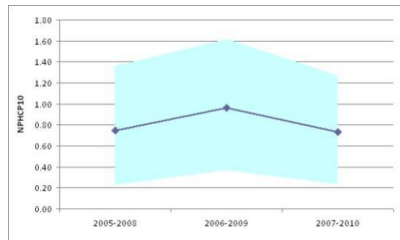
*Basic statistics*

Number of publications (P)	125
Number of citations (TCS)	657
Number of citations per publication (MCS)	5.29
Percentage of uncited publications	23%
Field-normalized number of citations per publication (MNCS)	.91
Field-normalized average journal impact (MNJS)	1.24
Field-normalized proportion highly cited publications (top 10%)	.68
Internal coverage	.89

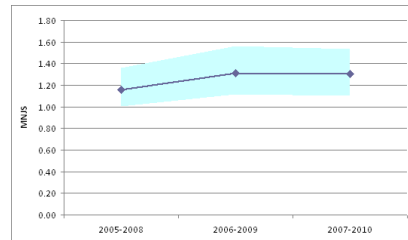
*Trend analyses*



MNCS

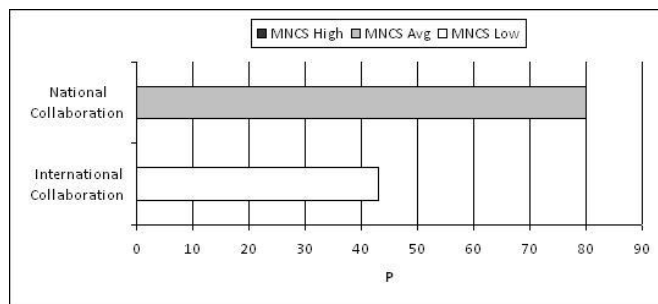


THCP10



MNJS

*Collaboration*



Performance (MNCS) by collaboration type

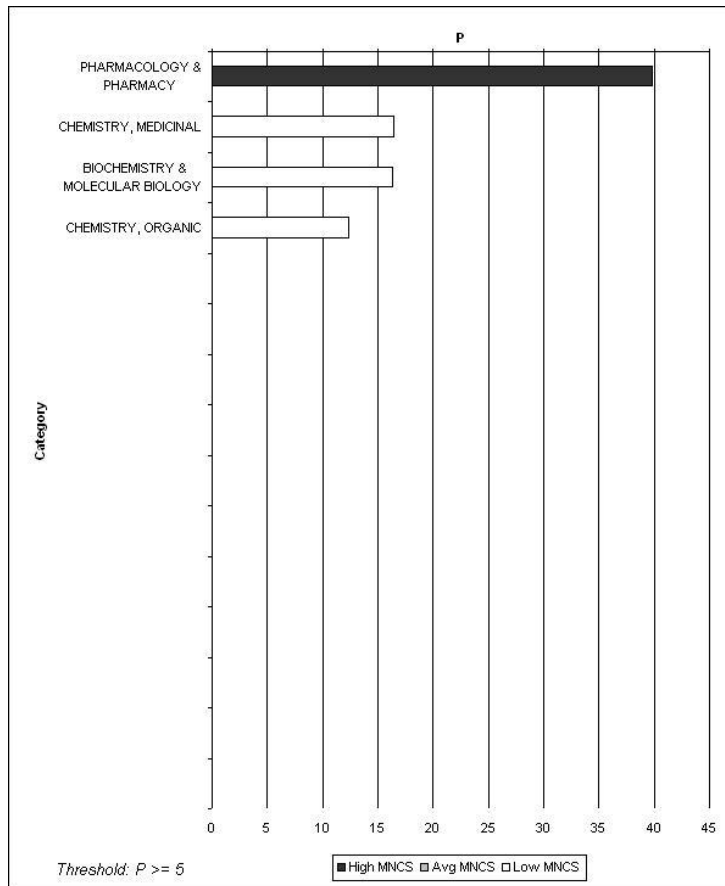




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