➢ Practical information

Place

The course takes place at 'Het Pand', Onderbergen 1, 9000 Ghent in auditorium Rector Blancquaert.

Time

Each session starts at 9 am and lasts till 1 pm with a coffee break in between.

Schedule

- 28/5: Computational Structural Chemistry
- 11/6: Quantum Chemistry
- 18/6: Protein Structure Determination
- 25/6: Protein Structure Based Drug Design
- 2/7: Property Based Drug Design

All dates mentioned above are Tuesdays.

Lecturers

The lecturers in this course, all experts in the topics they will discuss, include:

- Prof. dr. P.Bultinck (RUG, Theoretische chemie)
- Dr. H. De Winter (Janssen Pharmaceutica)
- Dr. W. Langenaeker (Janssen Pharmaceutica)
- Prof. dr. J. Tollenaere (UU, Computationele Medicinale Chemie)

More detailed information about ICES, 'Het Pand', itineraries, the specific topics that will be discussed and the curriculum and research of the lecturers can be found at the ICES site:
http://allserv.rug.ac.be/~shoste/ICES/

➢ Registration fees

Registration is possible through use of the enclosed enrolment form.

Payment due within 30 days following receipt of invoice	Normal price pp.	Price pp. if 3 or more people from the same company enrol together (-20%)*
Industry	600 €	480 €
Civil servant/Teacher (75%)	450 €	360 €
Student (50%)	300 €	300 €

* This reduction does not apply to students.

The registration fee includes notes, lectures, coffee, use of the auditoria and insurance.

Cancelling is possible in writing until ten days before the start of the module, in which case 25% of the registration fee will be retained. In case of cancellation within 10 days before the start of the course the full registration fee is due.

➢ For any further information

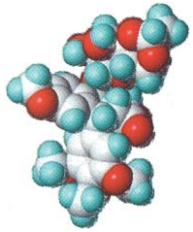
For more information about this and other ICES courses:

RUG – ICES, Krijgslaan 281, S3, 9000 Ghent, Belgium
Phone: +32 (0)9 264 44 26 Fax: +32 (0)9 264 49 83
E-mail: Heidi.DeDobbelaere@rug.ac.be or
Dana.Duprez@rug.ac.be
Url: http://allserv.rug.ac.be/~shoste/ICES/

COURSES TO COME:
Fall 2002: Course in **Bio-informatics** (2nd ed.)
Fall 2002 – Spring 2003: Courses in **Statistics**

ices

Institute for Continuing Education in Science



Computational Medicinal Chemistry

Faculty of Science

UNIVERSITEIT GENT

➢ Introduction

Medicinal chemistry is the branch of chemistry in which chemistry is used to gain insight in the chemical backgrounds of medicinal observations and to achieve certain medicinal goals and objectives. Admittedly, this is a broad definition, but as such embraces the very diverse set of domains of research currently associated to medicinal chemistry. Examples are drug discovery and molecular design, combinatorial chemistry, organic synthesis, pharmacology and biochemistry.

In recent decades, computational chemistry has attracted a great deal of attention. A rigorous definition of computational chemistry can hardly be made. It may be defined as the application of "computing" in chemistry. It then involves an enormous number of techniques, including e.g. data collection and handling, and analysis of experimental observations. Alternatively, computational chemistry is often identified as a subfield of theoretical chemistry, attempting to solve chemical problems using computations or calculations. Computational chemistry thus contains techniques such as computational quantum chemistry, force field calculations and molecular dynamics…

Computational chemistry has evolved into an important field within medicinal chemistry. In drug design e.g., computational chemical techniques are used routinely to identify underlying reasons for observed chemical reactivity, or to assess the probability of a molecule to exhibit certain desired properties.

When applied to medicinal chemistry, a vast array of computational techniques is used. Some of which are clearly geared almost solely to application in medicinal chemistry, yielding an active field of research in its own right: Computational Medicinal Chemistry.

Late spring 2002: Morning course in Computational Medicinal Chemistry

➢ Aims

A course on Computational Medicinal Chemistry can hardly address all different subfields of Computational Medicinal Chemistry. In the present course we will consider the subfields of computational structural chemistry, computational quantum chemistry, protein structure, protein structure based drug design and QSAR.

In the first session computational structural chemistry will be addressed as a set of techniques used to obtain three-dimensional structures of molecules from simple molecular representations, in addition conformational analysis with emphasis on force field techniques will be covered.

The session on computational quantum chemistry will address wave function based quantum chemistry including the basic aspects of doing quantum chemical calculations as well as Density Functional Theory including molecular reactivity descriptors.

Protein structure elements and folding will be the main subject of the third session, ...

... and in the session on protein based drug design topics such as docking of ligands in a receptor and scoring the interactions will be addressed.

Some aspects of ADME/Tox will be discussed in the final session on QSAR, together with classical QSAR and an introduction to quantum chemistry based QSAR techniques.

➢ Course organisation

This course will consist of 5 sessions each covering one of the aspects of Computational Medicinal Chemistry described above. It is organized by ICES under the joint scientific supervision of Prof. Dr. Jan Tollenaere, former head of the Theoretical Medicinal Chemistry group at Janssen Research Foundation and Professor of Computational Medicinal Chemistry at Utrecht University and Prof. Dr. Patrick Bultinck from the Theoretical Chemistry group at Ghent University. Experts from both industry and academia will give lectures.

➢ Intended public

The course is aimed at researchers in both industry and academia wishing to gain some knowledge on or improve their knowledge of the techniques used in Computational Medicinal Chemistry, the capabilities of the techniques, and the role of the different techniques in modern medicinal chemical research. The subjects discussed in the lectures may also be of general interest to other people from different branches of chemistry such as pharmacy, and other related disciplines …

➢ Required knowledge

The lectures are organised to be as self-contained as possible, starting at a basic level of theory, but addressing more involved techniques afterwards. Basic knowledge of terms used in computational chemistry is an advantage, as well as basic chemical, physical and medicinal chemical knowledge.

➢ Exam

At the end of the course participants get the opportunity to take a test. Participants who succeed in this exam receive a certificate of Ghent University.