

Medicinal Chemistry

Objectives

At the end of the course, participants will have gained:

An understanding of how biological disease targets are selected.

An insight in to the terms, definitions and analysis methods used by medicinal chemists in the pharmaceutical industry.

An introductory knowledge of the Pharmacokinetics and ADME (Absorption, Distribution, Metabolism and Excretion) and how physicochemical properties influence absorption

An introduction to the use of computational chemistry including pharmacophore generation, virtual screening and library design.

An overview of safety assessment and of chemical structure and safety

Outline

Introduction: Overview of drug discovery process, target selection in the post-genomic era

Introduction to Medicinal Chemistry, definitions, QSAR studies, drug receptors, Hansch Analysis, physico-chemical properties, Topliss Tree

Physico-chemical properties of drugs

Implications for Absorption

Lead generation approaches

Lead generation using computational techniques: molecular recognition, structure- and ligand-based virtual screening, success stories

Molecular diversity and combinatorial design

Pharmacokinetics and ADME with examples

Introduction to Lead Optimisation, Case Studies

Overview of some of the reasons for project failure, of safety, in particular to its relationship to chemical structure and of critical issues in Drug Development

Intellectual property issues related to drug discovery

What happens next? - a (very) brief overview of process development issues

Tutors

Dr David Clark is Director of Computer-aided Drug Design (CADD) and Information Services and was a founding scientific team member of Argenta Discovery in 2000. David began his career working for Proteus Molecular Design for 3 years where he was involved in developing software for de novo ligand design and protein-ligand docking. He then spent 4 years working in the CADD group of Aventis/Rhone-Poulenc Rorer before joining Argenta. David is a graduate of the University of Oxford where he studied chemistry. His post-graduate studies (MSc, PhD) were carried out at the Department of Information Studies at University of Sheffield under the supervision of Professor Peter Willett. In 2003, David was the recipient of the Corwin Hansch award, which is presented annually by the QSAR and Modelling Society.

Dr David Horwell graduated from London University before undertaking his PhD in organic heterocyclic chemistry at Leicester University with Professor C W Rees, CBE, FRS. He then carried out post-doctoral research in Canada (National Research Council, Ottawa), Florida (Gainesville) and at Imperial College, London. This was followed by a research career in the pharmaceutical industry with Eli Lilly, Parke-David, Warner-Lambert and Pfizer. David is the recipient of the 1998 Royal Society award for Medicinal Chemistry. He has been a Visiting Professor at The University of East Anglia for over 10 years and accepted the appointment of Chair of Medicinal Chemistry in September 2001 and now works as a freelance consultant in medical chemistry.

Medicinal chemists need to understand the relationship between chemical structure and the physical properties of molecules and how this translates into compound stability and the interaction of the molecule with biological structures.

These biological targets include proteins, lipids, nucleic acids and cell membranes. Interaction of the molecules with these targets affects the distribution of the compound in biological systems and modulates biological function.

To do this successfully the medicinal chemist needs to be aware of how target selection is carried out and how this affects lead generation. The medicinal chemist needs knowledge of structure property relationships, the physico-chemical properties of drugs and how these molecules interact with the body - pharmacokinetics and **ADME** (Absorption, Distribution, Metabolism and Excretion).

The course also includes an overview of the use of computational chemistry in virtual screening and library design. The lectures are backed up by a number of case studies and tutorial sessions, which involve the participants in using the concepts discussed.

Dr Geoff Lawton was formerly the Vice President Chemistry and Preclinical Sciences at Roche Bioscience, Palo Alto, California and has extensive experience of new medicine discovery and early development. In 2001 he became an independent consultant in all aspects of drug discovery from target identification, through lead finding and optimisation to drug candidate selection and evaluation. He is currently Research Director at Lectus Therapeutics.

Dr Nigel Rogers was formerly Director of Pre-clinical Science at Roche Discovery Welwyn and was instrumental in introducing new early ADMET approaches to enable better selection and design of compounds in Lead Optimisation. Nigel has also extensive experience of the process from Lead Identification through to NDA filing with responsibilities including project management, regulatory affairs and leadership of several projects. Nigel began his career at Roche as a Medicinal Chemist and continues to have a strong interest in the relationship of chemical structure to ADMET properties. He is now an independent consultant providing advice to the Pharma Industry.

Dr Will Watson his PhD in Organic Chemistry from the University of Leeds in 1980. He joined the BP Research Centre at Sunbury-on-Thames and spent five and a half years working as a research chemist on a variety of topics including catalytic dewaxing, residue upgrading, synthesis of novel oxygenates for use as gasoline supplements, surfactants for use as gasoline detergent additives and non-linear optical compounds. In 1986 he joined Lancaster Synthesis and during the next 7 years he was responsible for laboratory scale production and process research and development to support Lancaster's catalogue, semi-bulk and custom synthesis businesses. In 1993 he was appointed to the position of Technical Director, responsible for all Production (Laboratory and Pilot Plant scale), Process Research and Development, Engineering and Quality Control. He helped set up and run the Lancaster Laboratories near Chennai, India and had technical responsibility for the former PCR laboratories at Gainesville, Florida. He joined Scientific Update as Technical Director in May 2000. He has revised and rewritten the "Chemical Development and Scale Up in the Fine Chemical & Pharmaceutical Industries" course and gives this course regularly around the world. He has been instrumental in setting up and developing new courses such as "Interfacing Chemistry with Patents" and "Making and Using Fluoroorganic Molecules". He is also involved in an advisory capacity in setting up conferences and in the running of the events. He is active in the consultancy side of the business and sits on the Scientific Advisory Boards of various companies. He can be contacted by email at: will@scientificupdate.co.uk

Who Should Attend?

Young chemists who have just started in industry as medicinal chemists

Experienced medicinal chemists who wish to gain additional knowledge on how to obtain compounds with optimal drug-like properties and get up to date with the latest thinking.

Chemists from other areas of Research and Development who would like to gain an appreciation of the processes and drivers involved in drug discovery

Students who are planning a career in industry and can obtain company sponsorship

Fees

Fee includes lunch & refreshments, course dinner and course manual.

Accommodation

Scientific Update use high quality venues around the world. Preferential room rates including bed & breakfast are usually available.

Please check the Course Schedule on our website for venues, dates and availability.