



«ETTORE MAJORANA» FOUNDATION AND CENTRE FOR SCIENTIFIC CULTURE
TO PAY A PERMANENT TRIBUTE TO GALILEO GALILEI, FOUNDER OF MODERN SCIENCE
AND TO ENRICO FERMI, THE "ITALIAN NAVIGATOR", FATHER OF THE WEAK FORCES



INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

55th Course:

STRUCTURAL DRUG DESIGN 2020: BIOLOGY, CHEMISTRY AND COMPUTERS

ERICE-SICILY: 29 MAY – 6 JUNE 2020

Sponsored by the: • European Crystallographic Association • International Union of Crystallography
• Italian Ministry of Education, University and Scientific Research • Sicilian Regional Government

PROGRAMME AND LECTURERS

Historical perspective

• T.L. BLUNDELL, Cambridge University, UK

General crystallography

• C. LESBURG, MSD, Boston, MA, USA

CryoEM in drug discovery

• G. SCAPIN, MSD, Kenilworth, NJ, USA

1) High-throughput and automation

2) Measuring binding

• F. von DELFT, Diamond Light Source, Oxford, UK

1) Room temperature crystallography

2) Allostery

• J. FRASIER, UCSF, San Francisco, CA, USA

Introduction to NMR

• L. BANCI, Florence University, IT

NMR methods

• B. DAVIS, Vernalis, Cambridge, UK

Rationalising biomolecular interactions

• R. WADE, Heidelberg University, DE

1) Bioinformatics

2) Intro to biologics

• C. DEAN, Oxford University, UK

Data integration & pharmacology

• A. BRADLEY, Exscientia, Oxford, UK

Target engagement by MS

• J. TAUTON, UCSF, San Francisco, CA, USA

Rational design

• S. J. FLEISHMAN, Weizmann Institute, IL

Developability / Exp techniques

• O. OBREZANOVA, Lonza, Manchester, UK

Small-molecule chimeras

• J. WILLIAMS, City of Hope, Duarte, CA, USA

Drug discovery and development case study

• S. JACOB, Novartis, CH

Drug discovery and development case study 2

• G. McGAUGHEY, Vertex, Boston, MA, USA

Drug discovery and development case study 3

• E. ARNOLD, Rutgers University, Piscataway, NJ, USA

Docking /Free energy calculation / MD

• U. ROETHSBERGER, EPF, Lausanne, CH

Enumeration /Synthesis space

• J.P. EBEJER, Malta University, Malta

Modulators of protein function

• G. KLEBE, Marburg University, DE

PURPOSE OF THE COURSE

The past several years have produced transformations both in the long term management of chronic diseases and in the treatment of illnesses that previously seemed intractable. Nevertheless, understanding and managing human health remains one of the most challenging aspects of our society. One fundamental problem is the lack of a full comprehension of the underlying biology of healthy and diseased states. While structural information is still applied at different stages of the drug design process, especially atomic understanding during drug optimization, the focus has now decisively moved earlier, to providing tools for the understanding of the disease biology. This has resulted in traditional structural biology techniques being thoroughly integrated with other disciplines, including biophysics, informatics, biology and chemistry. In particular, the continuously evolving experimental and computational techniques, the success of the entire process depends on proper management of the increasing complexity, diversity and volume of data generated. The purpose of the course is to provide the students with: a) an overview of the current structural and biophysical techniques used in the field; b) the use of informatics tools in drug discovery; c) the evolving role of chemistry in drug design and biology understanding; and d) an introduction to biologics and their applications. Several case studies will be presented to highlight the different topics. Hands-on workshops and tutorials will complement the lectures.

APPLICATIONS

Interested candidates should register by 30th November 2019 using the form available at the URL <http://erice2020.azuleon.org> or by writing to the Executive Secretary of the International School of Crystallography:

- Dr. Annalisa Guerri
University of Florence Tel: +39.055.4573429
50019 Sesto Fiorentino, Italy email: annalisa.guerri@unifi.it

Please include the following information in your application:

- Your full name(s), age, gender, citizenship;
- Your postal address, phone, fax, electronic mail;
- Your present academic position and scientific interests;
- The title or abstract of a scientific contribution to the poster session(s) which might be included in the programme.

More information about the International School of Crystallography can be found on the WWW at the following address:

<http://www.crystalerice.org>

• PLEASE NOTE

Participants must arrive in Erice no later than 8 p.m. on 29th May 2020.

POETIC TOUCH

According to legend, Erice, son of Venus and Neptune, founded a small town on top of a mountain (750 metres above sea level) more than three thousand years ago. The founder of modern history — i.e. the recording of events in a methodic and chronological sequence as they really happened without reference to mythical causes — the great Thucydides (~500 B.C.), writing about events connected with the conquest of Troy (1183 B.C.) said: «After the fall of Troy some Trojans on their escape from the Achaean arrived in Sicily by boat and as they settled near the border with the Sicilians all together they were named Elymi: their towns were Segesta and Erice.»

This inspired Virgil to describe the arrival of the Trojan royal family in Erice and the burial of Anchises, by his son Aeneas, on the coast below Erice. Homer (~1000 B.C.), Theocritus (~300 B.C.), Polybius (~200 B.C.), Virgil (~50 B.C.), Horace (~20 B.C.), and others have celebrated this magnificent spot in Sicily in their poems. During seven centuries (XIII-XIX) the town of Erice was under the leadership of a local oligarchy, whose wisdom assured a long period of cultural development and economic prosperity which in turn gave rise to the many churches, monasteries and private palaces which you see today.

In Erice you can admire the Castle of Venus, the Cyclopean Walls (~800 B.C.) and the Gothic Cathedral (~1300 A.D.). Erice is at present a mixture of ancient and medieval architecture. Other masterpieces of ancient civilization are to be found in the neighbourhood: at Motya (Phoenician), Segesta (Elymian), and Selinunte (Greek). On the Aegadian Islands — theatre of the decisive naval battle of the first Punic War (264-241 B.C.) — suggestive neolithic and paleolithic vestiges are still visible: the grottoes of Favignana, the carvings and murals of Levanzo.

Splendid beaches are to be found at San Vito Lo Capo, Scopello, and Cornino, and a wild and rocky coast around Monte Cofano: all at less than one hour's drive from Erice.

More information about the «Ettore Majorana» Foundation and Centre for Scientific Culture can be found on the WWW at the following address:
<http://www.ccsem.infn.it>

Applicants may be able to apply for partial financial support. Please visit www.crystalerice.org to view the full eligibility criteria.

Young researchers should include in their application a list of no more than five scientific publications that they have authored, and a letter of recommendation from their supervisor or from a senior scientist, that justifies any support that the researcher requests.

In order to reflect the multi-disciplinary nature of the Course, priority will be given to applicants who have an appropriate scientific discipline, a good publication rate and a strong correspondence between their current research interest and the topics covered by the school.