



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



INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

58th Course: STRUCTURAL DRUG DESIGN 2023: BIOLOGY, CHEMISTRY AND COMPUTERS

ERICE-SICILY: 2 – 10 JUNE 2023

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. LESBÜRG, Odyssey TX, Cambridge, MA, US

CryoEM in drug discovery

- G. SCAPIN, Nanoimaging Services, Woburn, MA, US

1) High-throughput and automation

2) Measuring binding

- F. von DELFT, Diamond Light Source, UK

Allosteric & dynamics

- J. FRASER, UCSF, San Francisco, CA, US

1) Target selection

2) Project moonshot

- A. von DELFT, Oxford University, UK

Biologics developability

- R. BUICK, Fusion Antibodies, Belfast, IR

NMR methods

- B. DAVIS, Vernalis, Cambridge, UK

Rationalising biomolecular interactions

- R. WADE, Heidelberg University, DE

1) Machine learning in drug discovery

2) Intro to biologics

- C. DEAN, Oxford University, UK

1) Data integration in pharmacology

2) Compound design

- A. BRADLEY, Exscientia, Oxford, UK

Drug discovery and development case study 4

- J. PETERSEN, Astrazeneca, SE

Rational design

- S. J. FLEISHMAN, Weizmann Institute, Rehovot, IL

Small molecules chimeras

- J. WILLIAMS, City of Hope, Duarte, CA, US

Drug discovery and development case study 4

- S. JACOB, Novartis, Basel, CH

Drug discovery and development case study 5

- G. McGAUGHEY, Vertex, Boston, MA, US

Drug discovery and development case study 6

- E. ARNOLD, Rutgers University, Piscataway, NJ, US

Accelerating Drug discovery

- A. KOTECHA, ThermoFisher Scientific, Waltham, MA, US

Protein design and modeling / AlphaFold

- C. OUTERIAL, Oxford University, UK

Crystal structure prediction

- A. SHEIKH, AbbVie, Chicago, IL, US

In Silico SB optimization

- E. DAVIS, Schrodinger, US

Protein conformational landscapes

- M. FISCHER, St. Jude Hospital, Memphis, TN, US

PURPOSE OF THE COURSE

The past two years have been transformational in showing how the medical and scientific communities can respond to acute health threats: the worldwide collaboration of scientists from all fields of biology, chemistry and structural sciences delivered results at previously unseen speed. Nevertheless, understanding and managing all aspects of human health remains one of society's biggest challenges, and this in turn requires a robust understanding, currently still highly incomplete, of the underlying biology and healthy and diseased states. Structural information illuminates and accelerates all aspects of this drug design process, but the focus has remained decisively on the earlier stages, to providing tools for the understanding of the disease biology.

Moreover, traditional structural biology techniques have now been thoroughly integrated with other disciplines, including biophysics, informatics, biology and chemistry. This continuous evolution means that 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 13rd December 2022 using the form available at the URL <http://erice2023.azuleon.org> or by writing to the Executive Secretary of the International School of Crystallography:

Dr. Annalisa Guerri
University of Florence
50019 Sesto Fiorentino, Italy

Tel: +39.055.4573429
email: annalisa.guerri@unifi.it

Please include the following information in your application: i) Your full name(s), age, gender, citizenship; ii) Your postal address, phone, fax, electronic mail; iii) Your present academic position and scientific interests; iv) The title or abstract of a scientific contribution to the poster session(s) which might be included in the programme. Applicants may be able to apply for partial financial support. Please visit www.crystalalice.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.

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 methodical 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>

More information about the International School of Crystallography can be found on the WWW at the following address: <http://www.crystalalice.org>

• PLEASE NOTE

Participants must arrive in Erice no later than 8 p.m. on 2nd June 2023.