



ETHCSTWIN Summer School 2025

14-18 July 2025, Athens, Greece

Dept of Pharmacy, Lab of Pharmacognosy & Chemistry of Natural Products

Ethnopharmacology and Artificial Intelligence in Drug Discovery

Monday, 14 th July 2025	
15 ⁰⁰ -16 ⁰⁰	Presentation of ETHCSTWIN project Prof. Nektarios Aligiannis, Lab. of Pharmacognosy & Natural Products Chemistry, Dept of Pharmacy, NKUA / Coordinator of ETHCSTWIN project
16 ⁰⁰ -17 ⁰⁰	The study of the vascular flora of Greece: from the foundation of the modern Greek state to the present day. Historical review, phytogeography, endemic, rare and endangered plants, threats and conservation status Dr Ioannis Bazos, Section of Ecology & Systematics, Dept of Biology, NKUA
18 ⁰⁰ -19 ³⁰	Guided tour of the Botanical Garden Julia & Alexander N. Diomedes *

Tuesday, 15 th July 2025	
	Session 1. Ethnobotanical studies
9 ⁰⁰ -10 ³⁰	Visit to the Botanical Museum, NKUA
10 ³⁰ -11 ⁰⁰	Coffee Break
11 ⁰⁰ -12 ⁰⁰	Botanical and social scientific methods in field ethnopharmacology Prof. Andrea Pieroni, University of Gastronomic Sciences, Pollenzo, Italy
12 ⁰⁰ -13 ⁰⁰	Plants, People, and Shared Heritage: A unique experience on a Comparative Ethnobotanical study of Greek, Aromanian and Albanian Communities Dr Eva Dina, Lab. of Pharmacognosy & Natural Products Chemistry, NKUA
13 ⁰⁰ -14 ⁰⁰	Lunch Break
14 ⁰⁰ -15 ⁰⁰	Botanical Methods in Field Ethnopharmacology Prof. Avni Hadjari, University of Pristina, Kosovo
15 ⁰⁰ -15 ¹⁵	Peeling back the layers: Targeting, extraction and analysis of ethnobotanical data from the Balkans and beyond related to skin disorders Ioanna Maltezou, Lab. of Pharmacognosy & Natural Products Chemistry, NKUA
15 ¹⁵ -15 ³⁰	Integrating ethnobotanical knowledge in the study of gynaecological diseases: A data driven perspective through the eyes of an undergraduate student. Konstantinos Georgoulas, Lab. of Pharmacognosy & Natural Products Chemistry, NKUA
15 ³⁰ -16 ⁰⁰	The Power of Science: Bridging Traditional Knowledge and Modern Informatics Dr Mousaab Alrhoun, Faculty of Science and Technology, University of Bolzano
16 ⁰⁰ -17 ⁰⁰	Ethnobotanical Lab

Wednesday, 16 th July 2025	
	Session 2. Historical and Folklore Archives as sources of traditional therapeutic knowledge
9 ³⁰ -10 ³⁰	Premodern medical texts as sources of ethnopharmacological studies: Challenges and Future Prospects Assoc. Prof. Petros Bouras-Vallianatos, Department of History & Philosophy of Science, NKUA
10 ³⁰ -11 ⁰⁰	Coffee Break
11 ⁰⁰ -12 ⁰⁰	From <i>materia medica</i> to <i>chymia</i>: Greek Alchemy and Its Affinity with the Pharmacological Tradition Gerasimos Merianos, Senior Researcher, Institute of Historical Research, National Hellenic Research Foundation
12 ⁰⁰ -12 ³⁰	From manuscripts to editions: Making use of reliable textual sources Assoc. Prof. Petros Bouras-Vallianatos, Dept of History & Philosophy of Science, NKUA
12 ³⁰ -13 ³⁰	Lunch Break
13 ³⁰ -14 ³⁰	Ethnographic texts as sources of ethnobotanical information: An introduction. Assoc. Prof. Vassiliki Chryssanthopoulou, Department of Philology, NKUA
14 ³⁰ -15 ⁰⁰	Qualitative data mining from folklore archives in ethnobotanical contexts: Methodology, challenges and potential applications for ethnopharmacology Panagiotis Pozoglou, Department of Philology, NKUA
16 ⁰⁰ -18 ⁰⁰	Visit to the Benaki Museum

Thursday, 17 th July 2025	
	Session 3. Computer Science
9 ³⁰ -10 ³⁰	Resources for ethnobotany and ethnopharmacy: integration in ETHCSTWIN and how to use it Dr Christian Ebeling, Fraunhofer Institute for Algorithms and Scientific Computing
10 ³⁰ -11 ⁰⁰	Coffee Break
11 ⁰⁰ -12 ⁰⁰	A brief history of natural language processing - TLDR: from AST to LLM Dr. Marc Jacobs, Fraunhofer-Institute for Algorithms and Scientific Computing
12 ⁰⁰ -13 ⁰⁰	Managing and Analyzing Textual Data: An Algorithmic and Computational Systems View Dimitrios Gunopulos, Dept of Informatics and Telecommunications, NKUA
13 ⁰⁰ -14 ⁰⁰	Lunch Break
14 ⁰⁰ -15 ⁰⁰	Managing Ethnobotanical Data: Bridging Traditional Knowledge and Modern Data Science Vijay Ingalalli, PangeaBio
15 ⁰⁰ -18 ⁰⁰	Computer Science Lab: Introduction to Python programming: analyzing ethnobotanical and pharmaceutical data Dr Christian Ebeling, Fraunhofer Institute for Algorithms and Scientific Computing

Friday, 18 th July 2025	
	Session 4. Ethnopharmacology: Past, Present and Future
9 ³⁰ -10 ³⁰	From Traditional Remedies to Molecular Leads: Ethnopharmacology in Natural Products-Based Drug Discovery Prof. Nektarios Aligiannis, Coordinator of ETHCSTWIN project, Lab. of Pharmacognosy & Natural Products Chemistry, NKUA
10 ³⁰ -11 ⁰⁰	Coffee Break
11 ⁰⁰ -11 ³⁰	Navigating Chemical Space: Integrating Global Databases into In-House Compound Curation for Computational and Experimental Pipelines Vasileios Kaintas, Lab. of Pharmacognosy & Natural Products Chemistry, NKUA

11 ³⁰ -12 ¹⁵	Decoding Plant Chemistry with Mass Spectrometry: From Data Analysis to Molecular Networking Dr Alexandros Polyzois, Lab. of Pharmacognosy & Natural Products Chemistry, NKUA
12 ¹⁵ -13 ⁰⁰	NMR metabolic profiling in combination with chemometrics analysis for the discovery of bioactive natural products prior to isolation Dr Antigoni Cheilari, Lab. of Pharmacognosy & Natural Products Chemistry, NKUA
13 ⁰⁰ -14 ⁰⁰	Lunch Break
14 ⁰⁰ -16 ³⁰	Pharmacognosy Lab
16 ³⁰ -17 ³⁰	'From Traditional Knowledge to Modern Medicines: The Role of Ethnopharmacology in Drug Discovery' Manolis Mitakis, Head of Public Affairs & Communications at Boehringer Ingelheim
17 ³⁰	Summer School closing

***Tour of Diomedes Botanical Garden**

We invite all participants to join us for a guided visit to the Julia & Alexander N. Diomedes Botanical Garden, one of the most important in Greece. This is a unique opportunity to explore 2,500 species of plants.

 **Date:** Monday 14th July 2025

 **Location:** Chaidari, Athens

 **Time:** 6-8pm

 **Meeting Point:** Lab of Pharmacognosy and Chemistry of Natural Products (by bus to the garden)

 **Difficulty Level:** Easy walk, mostly shaded paths

 **What to Bring:** Hat & sun protection, Comfortable walking shoes, Water bottle

***Visit to the Botanical Museum, NKUA**

The Botanical Museum of the National and Kapodistrian University of Athens hosts an extensive collection of around 80,000 botanical specimens. These are divided into a historical herbarium (dating up to 1945) and a modern herbarium, which is continually updated and digitally catalogued. The Museum serves as a vital resource for botanical research and education.

 **Date:** Tuesday, 15th July 2025

 **Meeting point:** Lab of Pharmacognosy and Chemistry of Natural Products

 **Duration:** ~1 hour

***Visit to the Benaki Museum**

The Benaki Museum is one of Greece's leading cultural institutions, dedicated to showcasing the country's rich heritage across the centuries. During our visit, we will focus on the museum's manuscript collection, which includes rare historical texts, botanical and medical writings.

 **Date:** Wednesday, 16th July 2025

 **Meeting point:** Lab of Pharmacognosy and Chemistry of Natural Products
(transportation by bus No.608)

 **Duration:** ~2 hour

Ethnobotanical Lab (1hr)

Title: The Power of Science: Bridging Traditional Knowledge and Modern Informatics
Ethnobotany Lab – Data Analysis and Visualization

Summary: This hands-on lab introduces students to simple yet powerful digital methods for organizing, analyzing, and visualizing ethnobotanical data, without requiring programming skills. Participants will work with a real-world sample dataset that includes plant species, traditional uses, and cultural/geographic information. The session is designed for students and researchers from diverse backgrounds and will demonstrate how traditional knowledge can be enhanced through accessible digital tools

Requirements:

- A notebook/laptop (if available) with Excel or LibreOffice installed
- No prior technical skills needed, just curiosity and willingness to explore!
- All datasets and materials will be provided during the session

Topics:

1. Introduction to the dataset: short briefing on how ethnobotanical data is collected and structured.
2. Data organization and cleaning:
3. Visualization: creating simple bar charts, pie charts, and tables to explore the frequency of plant uses and cultural patterns.
4. Spatial analysis overview: optional basic mapping of plant locations using Google Maps or QGIS (no installation required; pre-prepared map examples can be shown).
5. Some advanced Analysis by R or SAS 9.4
6. Group reflection: discussion of observed patterns, challenges, and the value of digital methods in preserving and interpreting traditional knowledge.

Computer Science Lab (3hrs)

Title: Introduction to Python programming: analyzing ethnobotanical and pharmaceutical data

Summary: This lab will be a hands-on introduction into basic python programming. You will learn how to extract information from different resources. By using Jupyter notebooks we will analyzing several ethnobotanical data and creating statistics. With a graph library you will visualize your results in different charts and plots.

Requirements:

- Own notebook (Windows, MacOS or Linux)
- Programming skills are not required
- Instruction how to install Python, Visual Studio Code and Git will be send right before the lab starts

Topics:

1. Introduction into python
2. How to use Visual Studio Code (VSCode)
3. Simple scripts and Jupyter notebooks
4. Import data from a publication
5. Query data from ETHCSTWIN server
6. Using advanced pandas methods to analyze the data and create statistics
7. Creating different maps, charts and plots

Pharmacognosy Lab (2.5 h)

Title: From Plant to Profile – A Hands-On Exploration of Natural Products

Summary: This interactive lab introduces participants to the core techniques of natural product research and pharmacognosy. This session is ideal for researchers of all disciplines with an interest in drug discovery from natural sources.

Starting from raw plant material, participants will carry out a complete phytochemical workflow: extraction using solvents of different polarity, concentration using rotary evaporation (Rota vapor), and chemical profiling using modern analytical techniques such as HPTLC. The lab concludes by providing already acquired HPLC-DAD/ELSD, LC-MS and NMR profiling datasets, offering insight into how chemical fingerprints support the identification and quality control of bioactive compounds in medicinal plants.

Requirements:

- Lab coat and safety glasses
- No prior lab experience required – just curiosity and attention to detail!
- All materials and equipment will be provided

Topics:

- Introduction to plant selection and phytochemical workflow.
- Extraction of plant material using solvents of varying polarity.
- Evaporation and concentration using rotary evaporator (Rota vapor). Also, demonstration of lyophilizer and speed vacuum apparatuses.
- HPTLC: principles and hands-on application for phytochemical screening.
- HPLC-DAD/ELSD: chromatographic separation and interpretation of plant constituents.
- NMR & LC-MS: Discussion on handling NMR and LC-MS data.
- Group discussion: interpretation of profiles and their role in quality control and phytotherapeutic development.