Data Science for Chemists

17/06/2024 9h-12h (JSA) 1. Introduction to Data Science	Objective: This part is an introduction to different themes related to data science required for chemists We will take a look at different concepts related to data science • History of Data Science and computing • Computer Architecture and Systems • Major phases of data analysis • Algorithms for data acquisition and process control • Applications: sustainable cities, energy transitions
17/06/2024 14h-17h (OCA) 2. Internet of things	Objective: This part gives an introduction to different themes related to Internet of things required for chemists It will cover the following topics: • History of Internet of Things (IoT) • Definition of IoT • Applications: Industry 4.0, circular economy • IoT architectures • Fog/Edge/Cloud computing
18/06/2024 9h-12h (OCA) 3. Data acquisition protocols and technologies for IoT	Objective: This part presents data acquisition protocols and technologies for IoT We will take a look at the key concepts of IoT IoT Technologies Data acquisition protocols like SPI, I2C Sensors Actuators
20/06/2024 9h-12h (JSA) 4. Fundamentals of Programming	Objective: This part gives a general overview of programming in Python with the goal of using it for data analysis The student will be able to get an overview of • Fundamentals of Python programming • Manipulation of files, especially reading, writing and modifying text files and CSV/TSV and JSON files • Interaction with the user

	Data Analysis (basic) using built-in Python methods
24/06/2024 9h-12h (JSA) 5. Data Analysis and visualization	Objective: This part gives the fundamentals of data analysis and visualization It will cover the following topics Clustering algorithms Classification algorithms Linear regression models Recommender systems Visualization techniques
25/06/2024 9h-12h (OCA) 6. Practical session on Microcontrollers	 Objective: This part gives a hands-on experience on the microcontrollers The student will be able to perform the following Coding, compiling and flashing a firmware for microcontroller Interacting with sensors and actuators using SPI and I2C protocols Reading digital and analog measures
27/06/2024 14h-17h (JSA) 7. Data Mining	 Objective: This part gives an opportunity to the students to use data mining tools We will look at the following topics: Introduction of Python libraries like numpy, matplotlib and pandas Manipulating CSV and JSON files using the above libraries Data analysis Data visualization techniques for different types of data Clustering, classification and linear regressing using the library Scikit-learn.
28/06/2024 9h-12h (OCA) 8. Network protocols for IoT	Objective: This part gives an introduction to the network protocols for data communication We will cover the following topics Network protocols like LPWAN and WPAN Message exchange protocols like MQTT
01/07/2024 9h-12h (OCA) 9. Scaling up IoT	Objective: This part introduces ways to scale up the loT architectures

	The students will discover The challenges while scaling up IoT IoT Lab infrastructure
01/07/2024 14h-17h (JSA) 10. Machine Learning	Objective: This part gives an introduction to machine learning techniques We will cover the following topics Supervised, unsupervised and semisupervised learning Neural network models including single and multilayered perceptron Analysis of sensor data Image analysis Prediction Recognition of handwriting
02/07/2024 9h-12h (OCA) 11. Practical session on IoT-Lab	Objective: This part introduces ways to use message and network protocols for IoT lab The students will work on • LoRa WAN • MQTT
04/07/2024 9h-12h (JSA) 12.Big Data	Objective: This part will introduce the key concepts of Big Data Following are the topics covered in this module: • 5V of Big Data • Data storage of voluminous data, especially non-relational databases • Artificial Intelligence • Open databases and extraction of information
08/07/2024 9h-11h (OCA-JSA) Evaluation	Final exam of two hours based on all the topics covered in this module.
