Course unit English denomination	**Drug-receptor interactions: theory and techniques**
Teacher in charge (if defined)	DE FILIPPIS Vincenzo
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	09/2025
Course delivery method	☐ In presence ☐ Remotely ☒ Blended
Language of instruction	English
Mandatory attendance	☒ Yes (50 % minimum presence) ☐ No
Course unit contents	The course aims at providing the Ph.D. students of the School in Molecular Science an up-to-date overview of the theoretical approach in studying drug-receptor interactions and of the chemical, biochemical, and physical methods currently used for quantifying macromolecular interactions. 1) Generality on the structure and function of proteins as targets of drug activity: soluble receptors and nuclear receptors, membrane-bound receptors, G protein-coupled receptors, integrins, enzymes as key targets of drugs, DNA as a receptor for innovative drugs.2) Theoretical aspects for describing drug-receptor interactions: rigid-body mechanism, adaptive mechanism, population-shift mechanism, implications of receptor and ligand conformational flexibility in drug discovery. Analysis of binding data: Langmuir model of single binding, the tight- and slow-binding model, multiple equivalent and nonequivalent binding, and model for allosteric interactions. Derivation of thermodynamic quantities of ligand binding using the van't Hoff treatment. 2) Experimental methods to monitor and quantifying the strength of ligand-receptor interaction (a personal classification). • Molecular biology methods (two hybrid systems, enzyme-linked immunosorbent assays, microchips, and micro-arrays). • Chemical methods (affinity chromatography, size-exclusion chromatography; native electrophoresis, chemical crosslinking, 'native' mass spectrometry techniques and hydrogen-deuterium exchange mass spectrometry, HDX-MS) • Physical methods (equilibrium dialysis, ultracentrifugation at equilibrium, dynamic and static light scattering, surface plasmon resonance, calorimetric methods) • Spectroscopic methods (differential UV absorption and second derivative UV spectroscopy, far- and near-UV circular dichrosim, fluorescence spectroscopy, fluorescence anysotropy) • Biochemical methods (determination of the kinetic constants kcat and Km of enzyme activity, determination of the inhibition constant Ki of reversible competitive, non-competitive and incompetitive inhibitors). 3) Hands-on experience (4 hours): determination of binding constants by SPR, calorimetric and fluorescence techniques.

Learning goals	Knowledge: structure and function of biological molecules; basic principles of the most widespread physical and chemical methods useful for studying drug-receptor interactions. Skills: design of an experimental setup for measuring the affinity of a drug for the target receptor using fluorescence and SPR methods. Competencies: design of suitable strategies for identifying drug-receptor interactions and for the quantitative determination of drug-receptor affinity.
Teaching methods	**Frontal teaching**
Course on transversal, interdisciplinary, transdisciplinary skills	☒ Yes ☐ No
Available for PhD students from other courses	☒ Yes ☐ No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	max 3750 caratteri
Examination methods	**One-to-one talk on the theory and applications of the techniques studied during the course.**
Study material	**Slides/articles and registrations of the lessons provided by the teacher**
Additional information (not mandatory)	max 3750 caratteri