Master´s Degree in Pharmacological Research (2019-2020)

Subject: **DRUG DESING: FROM CLASSICAL TO "IN SILICO" (CODE-33207)**

- 2nd Semester-Week 1

Hour	Monday-6 January	Tuesday- 7 January	Wednesday-8 January	Thursday- 9 January	Friday- 10 January
9-10h			Drug design: General overview **Rafael León**		
10-11h			Classic Drug design: 2.1.- Drug targets 2.2.- Proteins: Structure and functions 2.3. Intermolecular forces **Cristobal de los Rios**	Classic Drug design: 2.5. Drug targets: Signal transduction and nucleic acids José Carlos Menéndez	3.7. Hit-to-lead and lead to drug optimization **José Carlos Menendez**
11-12h			Classic Drug design: 2.4. Drug targets: Enzymes **Cristobal de los Rios**	3.3. Hybridization 3.4. Bioisosteric modification of active compounds **Cristobal de los Rios**	3.8. ADME optimization **José Carlos Menéndez**
12-13h			Classic Drug design: 2.5. Drug targets: Receptors **Cristobal de los Rios**	3.5. Quantitative Structure-activity relationships 3.6. Target interactions-based optimization **Cristobal de los Rios**	4.1. Computer assisted drug design: Basics 4.2. Molecular and quantum mechanics **Federico Gago**
13-14h				3.1. Finding a lead compound 3.2. Active compounds-based drug design **Cristobal de los Rios**	4.3. Protein preparation and 3D pharmacophore preparation **Federico Gago**

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2nd Semester-Week 2

Hour	Monday- 13 January	Tuesday- 14 January	Wednesday-15 January	Thursday-16 January	Friday- 17 January
9-10h					
10-11h			4.5. Virtual screening and data analysis **Sonsoles Martín**	Presentations of manuscripts	Presentations of manuscripts
11-12h	4.4. Molecular docking and binding energy determination **Felipe Franco**		4.6. Molecular dynamics **Sonsoles Martín**		
15-16h	* **Practices** Drug design: **PDB Pymol**	* **Practices**: Drug design: **Molecular docking**	* **Practices**: Drug design: • **Molecular dynamics.** • **Virtual screening** • **Unbiased classical**	* **Practices**: Drug design: **Molecular dynamics: Complex and dynamics**	* **Practices:** Drug design: **Molecular dynamics: Complex and dynamics MD analysis**
16-17 h					
17-18 h					
18-19 h					