

# Center for Biological Research Margarita Salas (CSIC)

Ramiro de Maeztu 9, 28040 Madrid, Spain

## At a glance

- EU-OPENSREEN medicinal chemistry site with wide experience in structure based drug design (SBDD) and chemical genetics mainly for small heterocyclic compounds
- Synthetic chemistry designed to scale up the final pathways
- Hit-to-lead optimization beyond biological activity: looking for increase drug-like properties
- Virtual screening, computational chemistry and QSAR analysis included in our programs (drug discovery and drug optimization)
- More than six successful programs from the bench to the clinical trials

## Infrastructure and technical focus

- Synthetic and analytical capacity: hoods, lab space, microwave synthesizer, flash chromatography system, NMR, MS, HPLC/MS, elemental analysis
- ADME profile portfolio: solubility, PAMPA (BBB and oral absorption prediction) and microsomal stability
- Binding kinetics: Standard assays for kinases
- Chemoinformatics: work stations, computing clusters, and access to supercomputers clusters and scientific softwares



Prof. Dr. Ana Martínez (Head of Unit)

„Being part of EU-OPENSREEN reinforces the internationalization of CSIC and allows our laboratory to achieve relevance beyond our borders. We contribute with our knowledge in the field and help to find drug candidates that can reach clinical phases.“

## Projects past and present

**2020 - 2021 | CoV2Drugs** Target-and ligand-based drug repurposing to control SARS-CoV-2 pandemic [➔ Link](#)

**2018 - 2021 | ELA Madrid** Design and development of innovative drugs for the treatment of ALS [➔ Link](#)

**2017 - 2021 | DRIVE** Driving next generation autophagy researchers towards translation [➔ Link](#)

## Our science in selected publications

COVID-19: Drug Targets and Potential treatments  
[➔ Journal of Medicinal Chemistry \(2020\), 63, 12359–12386](#)

Motor neuron preservation and decrease in vivo of TDP-43 phosphorylation by protein CK-1 $\delta$  kinase inhibitor treatment  
[➔ Scientific Reports \(2020\), 10, Article number: 4449](#)

Benzothiazole-based LRRK2 inhibitors as Wnt enhancers and promoters of oligodendrocytic fate  
[➔ Journal of Medicinal Chemistry \(2020\), 63, 2638-2655](#)

Deciphering the enzymatic target of a new family of antischistosomal agents bearing a quinazoline scaffold using complementary computational tools  
[➔ Journal of Enzyme Inhibition and Medicinal Chemistry \(2020\), 35, 511-523](#)

## Further info and site-contact

**Prof. Dr. Ana Martínez:** [ana.martinez@csic.es](mailto:ana.martinez@csic.es) | +34 (0) 91 8373 112

**Website:** <https://www.cib.csic.es>

