ES | Medicinal chemistry site

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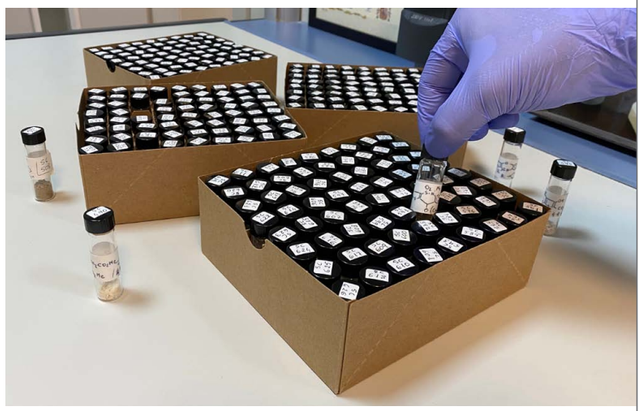
„Being part of EU-OPENSCREEN reinforces the internationalization of CSIC and allows our laboratory to achieve relevance beyond our borders. We contribute with our knowledge in the field and help to find drug candidates that can reach clinical phases.“

At a glance

- EU-OPENSCREEN medicinal chemistry site with wide experience in structure based drug design (SBDD) and chemical genetics mainly for small heterocylcic 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 successfull 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



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-1δ kinase inhibitor treatment
Scientific Reports (2020), 10, Article number: 4449

Benzothiazole-based LRRK2 inhibitors as Wnt enhancers and pomoters of oligodencrocytic 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

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