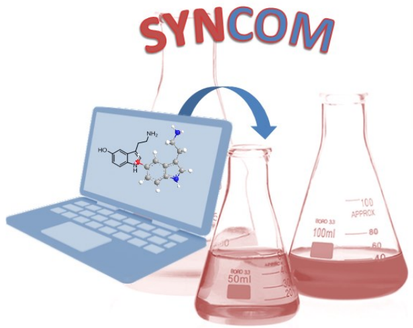
SYNCOM Group



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SYNCOM

ORGANIC SYNTHESIS AND COMPUTATIONAL CHEMISTRY LABORATORY

Research activity

The research group is focused on two key areas, synthetic organic chemistry and computational chemistry, which are highly complementary and in complete synergy with each other.

Organic Synthesis

It mainly concerns the Pharmaceutical field with the aim of creating new chemical entities endowed with biological and/or diagnostic activity which, in the future, can represent new leads and, from a more general perspective, identify new therapeutic prototypes. Furthermore, the research group is interested in the development of new chemical methodologies in the medicinal chemistry context.

Computational Chemistry

It essentially concerns the medicinal chemistry field and is focused on the study of the interaction between the drug and its macromolecular target

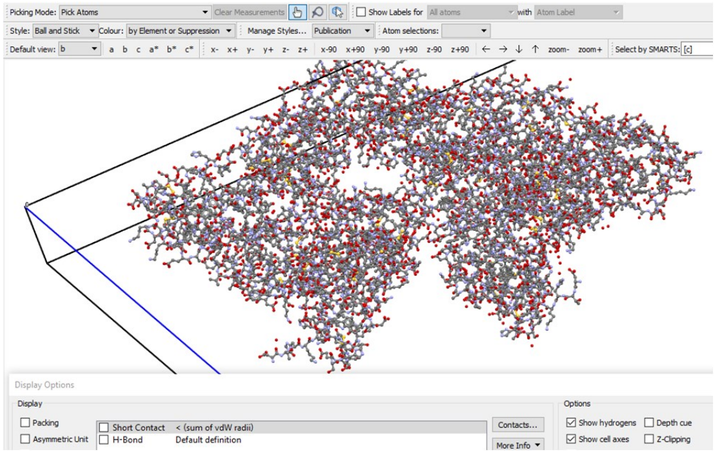
The **main lines of research** concern:

- Receptor modulators CB1, CB2, TRPA1, TRPV, GABAB, 5-HT3, CBR;
- Multitarget compounds with potential neurodegenerative activity;
- Compounds with antibacterial, antitubercular and antitumor activity;
- Photopharmacological therapy through the development of ligands with reversible photomodulatory biological activity (main targets ChE, MAO);
- Development of fluorescent markers.

The research group's skills involve:

•Design of new molecules of pharmaceutical interest;
•Modification of natural molecules of pharmaceutical interest;
•Creation of pharmacophore models to be applied in virtual screening ;
•Elaboration of receptor models;
•*In silico* evaluation of the chemical-physical properties of molecules;
•Application of Machine Learning (AI) algorithms to chemical problems;
•Organic synthesis;
•Purification and analysis of organic compounds;
•Experimental determination of the solubility and logP of organic molecules;

Images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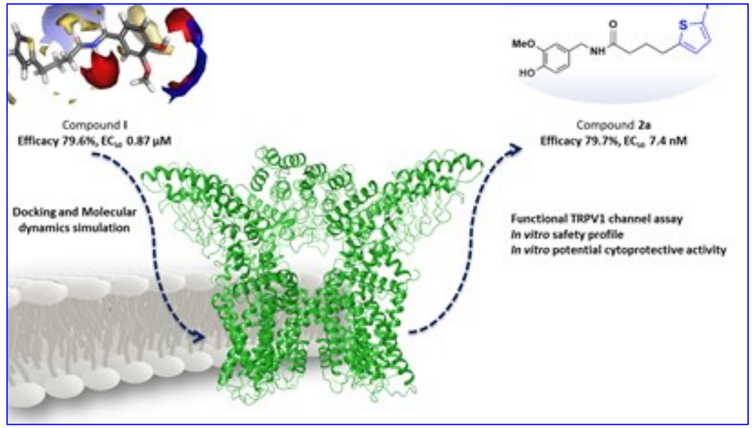
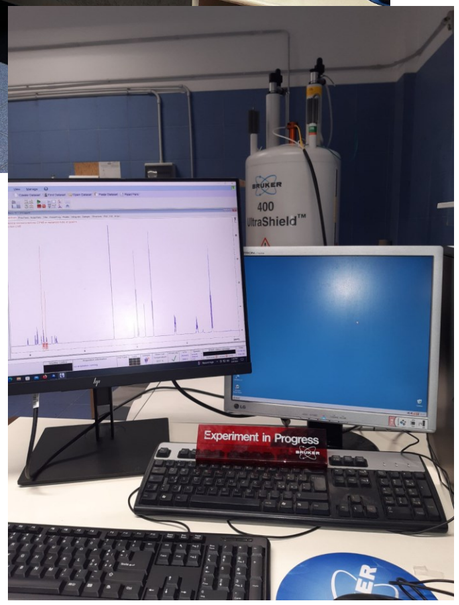

Compound I
Efficacy 79.6%, EC50 0.87 μM
Docking and Molecular dynamics simulation
MeO
HO
NH
O
S
Compound 2a
Efficacy 79.7%, EC50 7.4 nM
Functional TRPV1 channel assay
In vitro safety profile
In vitro potential cytoprotective activity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Experiment in Progress

Technologies and services

The group is equipped with state-of-the-art molecular modeling software suites and workstations. The unit also makes use of a high-performance computer cluster equipped with 640 Intel Skylake Gold processors, 3800 GB of RAM, 20 TB of storage, and 6 Nvidia V100 GPUs (21000 cuda cores in total). A fully equipped synthetic chemistry laboratory is available with a CEM Discover Synthesis Unit (CEM Corp, Mattnews, NC) and chemical analysis facilities including a Brucker Avance DRX-600/400 NMR spectrometer and a LC-MSD 110 series AGILENT with an electrospray interface, UV spectrometer Cary-60 Agilent, FT-IR Cary 630 among other. Moreover, the group has access to the MS Center equipped with latest generation HPLC/UHPLC systems and fully equipped Bruker timsTOF system for proteomics.

The **activities** that can be **provided to businesses** are:

- On-demand synthesis of new organic molecules
- Supply of organic molecules belonging to the internal chemotherapy library
- Purification, analysis and identification of organic molecules
- Processing of receptor models
- Development of pharmacophore models
- Docking
- Virtual screening of compound libraries

Applications and collaborations

Activities already carried out for companies.

The research group has experience of collaboration with pharmaceutical, diagnostic and cosmetic companies across the entire national territory and is available for the application of the following services:

- On-demand synthesis of new organic molecules of pharmaceutical interest
- Supply of organic molecules belonging to the internal chemotherapy library
- Structural and chemical-physical characterization of small organic molecules
- QSAR, 3D-QSAR and molecular modeling studies
- Investigation of pharmacological targets on request, from rational design to the synthesis of new bioactive molecules.
- Development of pharmacological tools in precision medicine.

For more information

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For more information

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