

CISUP

"Q EXACTIVE PLUS ORBITRAP" LABORATORY

(DEPARTMENT OF PHARMACY)

Management: Prof. Alessandra Braca

Head of laboratory: Dr. Marinella De Leo

Laboratory technician: Dr. Beatrice Muscatello

Laboratory web-page: <https://cisup.unipi.it/labs/orbitrap-q-exactive-plus/>

Location: Department of Pharmacy, Via Bonanno Pisano 33, second floor

Partial Activity Report 2022

In this partial report, the activities carried out in the "Q Exactive Plus Orbitrap Lab" during January-September 2022 are reported.

Laboratory implementation

As in previous years, the laboratory was implemented to cover analyses requested in different fields, as well as in metabolomics and proteomics.

The laboratory was further accessorized with:

- different UHPLC, micro- and nano-LC columns;
- solvents and standards;
- general lab equipment and consumables.

Laboratory users

An increasing number of requests by UNIFI Departments and external Research Institutes was registered during this year, indicating an increasing visibility of CISUP. Furthermore, different scientists were interested to include the equipment in starting projects.

The users of the laboratory include 24 research groups from 4 departments of the Pisa University (Department of Pharmacy; Department of Agriculture, Food and Environment; Department of Translational Medicine and New Technologies in Medicine and Surgery; Department of Earth Science), and 3 private Companies.

Many experiments are still in progress and scheduled for the next few months.

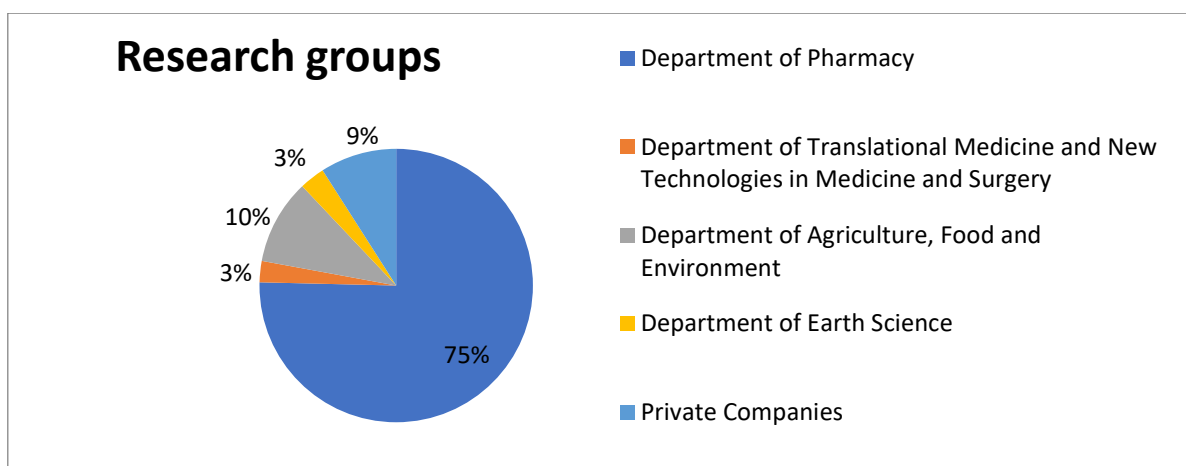


Fig. 1. Laboratory users

Hours worked and income

The total hours worked in January-September 2022 have been estimated ~700.

The total income is still in reporting, but it can be estimated ~20.000 €.

Maintenance and training

In addition to the weekly maintenance in house, the annual preventive maintenance visit was carried out in September for 3 consecutive days.

Products

Analyses performed at the Orbitrap lab covered a wide range of research topics in the field of chemistry, biochemistry, and drug discovery:

- structural determination of both natural and synthetic drugs
- chemical characterization and quantitative analysis of biomolecules in plant extracts, foods, and agro-food by-products
- quantitative analysis of drugs in cells and tissues
- quantitative analyses of endogenous substances in tissues
- chemical characterization of synthetic and natural polymers
- molecules structural study and fragmentation mechanism
- study and characterization of the adducts of pharmacologically active metallodrugs with biological targets
- determination of impurities
- monitoring of chemical reactions
- validation of analytical methods.

Obtained results were published in international journals, as listed below:

1. Bacci A., Corsi F., Runfola M., Sestito S., Piano I., Manera C., Saccomanni G., Gargini C., Rapposelli S. (2022). Design, synthesis, and *in vitro* evaluation of novel 8-amino-

quinoline combined with natural antioxidant acids. *Pharmaceuticals* 15, 688. DOI: 10.3390/ph15060688

2. Bononi G., Flori L., Citi V., Acciai C., Nocilla V., Martelli A., Poli G., Tuccinardi T., Granchi C., Testai L., Calderone V., Minutolo F. (2022). New synthetic analogues of natural polyphenols as sirtuin 1-activating compounds. *Pharmaceuticals* 15(3):339. DOI: 10.3390/ph15030339
3. Bononi G., Di Stefano M., Poli G., Ortore G., Meier P., Masetto F., Caligiuri I., Rizzolio F., Macchia M., Chicca A., Avan A., Giovannetti E., Vagaggini C., Brai A., Dreassi E., Valoti M., Minutolo F., Granchi C., Gertsch J., Tuccinardi T. (2022). Reversible monoacylglycerol lipase inhibitors: Discovery of a new class of benzylpiperidine derivatives. *J Med Chem* 65(10):7118-7140. DOI: 10.1021/acs.jmedchem.1c01806.
4. Boudermine S., Parisi V., Lemoui R., Boudiar T., Chini M.G., Franceschelli S., Pecoraro M., Pascale M., Bifulco G., Braca A., De Tommasi N., De Leo M. (2022). Cytotoxic sesquiterpenoids from *Ammoides atlantica* aerial parts. *J Nat Prod* 85(3):647-656. DOI: 10.1021/acs.jnatprod.1c01211
5. D'Angiolo M., De Leo M., Camangi F., Magliocca G., De Tommasi N., Braca A., Marzocco S. (2022). Chemical constituents of *Ulmus minor* subsp. *minor* fruits used in the Italian phytoalimurgic tradition and their anti-inflammatory activity evaluation. *Planta Med.* DOI: 10.1055/a-1787-1342. In press.
6. Di Stasi M., Donadio G., Bader A., De Leo M., Braca A. (2022). Two new triterpenes from *Commicarpus grandiflorus* (A. Rich.) Standl. aerial parts exudate. *Nat Prod Res.* DOI: 10.1080/14786419.2022.2063855. In press
7. Fabiano A., De Leo M., Cerri L., Piras A. M., Braca A., Zambito Y. (2022). Saffron extract self-assembled nanoparticles to prolong the precorneal residence of crocin. *J Drug Deliv Sci Technol* 103580. DOI: 10.1016/j.jddst.2022.103580.
8. Felice F., Cesare M.M., Fredianelli L., De Leo M., Conti V., Braca A., Di Stefano R. (2022). Effect of tomato peel extract grown under drought stress condition in a sarcopenia model. *Molecules* 27, 2563. DOI: 10.3390/molecules27082563.
9. Massai L., Cirri D., Marzo T., Messori L. (2022). Auranofin and its analogs as prospective agents for the treatment of colorectal cancer. *Cancer Drug Resist* 5(1):1-14. DOI: 10.20517/cdr.2021.71.
10. Politi M., Ferrante C., Menghini L., Angelini P., Flores G. A., Muscatello B., Braca A., De Leo M. (2022). Hydrosols from *Rosmarinus officinalis*, *Salvia officinalis*, and *Cupressus sempervirens*: Phytochemical analysis and bioactivity evaluation. *Plants* 11, 349. DOI: 10.3390/plants11030349

11. Robello M., Salerno S., Barresi E., Orlandi P., Vaglini F., Banchi M., Simorini F., Baglini E., Poggetti V., Taliani S., Da Settimo F., Bocci G. (2022). New antiproliferative agents derived from tricyclic 3,4-dihydrobenzo[4,5]imidazo[1,2- α][1,3,5]triazine scaffold: Synthesis and pharmacological effects. *Arch Pharm*, e2200295. DOI: 10.1002/ardp.202200295
12. Tolbatov I., Cirri D., Tarchi M., Marzo T., Coletti C., Marrone A., Messori L., Re N., Massai L. (2022). Reactions of arsenoplatin-1 with protein targets: A combined experimental and theoretical study. *Inorg Chem* 61(7):3240-3248. DOI: 10.1021/acs.inorgchem.1c03732.
13. Tremolanti C., Cavallini C., Meyer L., Klein C., Da Pozzo E., Costa B., Germelli L., Taliani S., Patte-Mensah C., Mensah-Nyagan A.G. (2022). Translocator protein ligand PIGA1138 reduces disease symptoms and severity in experimental autoimmune encephalomyelitis model of primary progressive multiple sclerosis. *Mol Neurobiol* 59(3):1744-1765. DOI: 10.1007/s12035-022-02737-2.