Molecular Horizon is an innovative start-up founded in 2017 and based in Bettona (PG), green heart of Italy.

The main research line addresses the strategic programme “Integrated platform for the research and development of innovative drugs for oncological and metabolic diseases”, presented by a consortium of Molecular Horizon and three other companies with the aim of bringing together the different but complementary competences of the participating companies in an integrated platform for the development of innovative molecules capable of opening new horizons for therapeutic treatments in the field of oncological and metabolic diseases.

The underlying strategy of the programme is based on the creation of a new and effective communication and collaborative research and development platform (Discovery Platform) that unites the partners’ competences for the development of new pharmacologically active molecules, in order to meet the medical needs linked to the study of the treatment of oncological and metabolic diseases. It thereby fully corresponds to the priority area of Life Sciences in the RIS3 Strategy of the Umbria Region and creates the first drug discovery specialized research cluster in Umbria.

This “Drug Design and Discovery” approach, represents one of the most fascinating and complex challenges in scientific endeavour whilst at the same time also being one of the most promising areas for innovation in research and development for new pharmaceutical products that can guarantee a better quality of life and scientific understanding for diseases that are not yet effectively treatable.

**OUR MISSION**

- development of software solutions for chemistry, pharmaceutical chemistry and biotechnology
- consultancy in the fields of chemometrics, drug design, and lipidomics.
- implementation of the project “Integrated platform for the research and development of innovative drugs for oncological and metabolic diseases”
The implementation of the project “Integrated platform for the research and development of innovative drugs for oncological and metabolic diseases” requires the constant and synergic integration of our three main research lines.

**Platform Design and Development**
Design and development of a technical and scientific platform for data storage and handling, databases query, and physical-chemical properties predictions accessible by all of the companies of the consortium thanks to cloud computing technology. A team of highly skilled informaticians, cheminformaticians and chemometricians, as well as researcher who understand biological and pharmaceutical meanings of experimental data work together for the completion of this goal.

**Technical Highlights:**
• Design of database for chemical structures, experimental data, spectral characterization (big data), metadata
• Integration of an high throughput platform for LCMS lipidomics and software for MetID and LipidID
• Developing of a cloud-area for the database
• Developing of a secure and encrypted access (both in download and upload) to the database from any electronic device and OS

**Lipidomics and Medicinal Chemistry**
Design and development of novel compounds. The chemical and pharmaceutical character of innovation is granted by a design step guided by lipidomics investigations on human microtissues. The completion of this step is promoted by the collaboration of the Department of Chemistry, Biology and Biotechnology of the University of Perugia.

**Technical Highlights:**
• Optimization of metabolism properties and early-toxicity tests of developed compounds
• High throughput lipidomic investigations by means of LCMS lipidomics, LipidID and MetID software
• Human microtissues experiments
• Multivariate statistical analysis and evaluation of the effect of the dosed compounds (end points) via lipidomic fingerprints comparison

**Drug Design and Molecular Modelling**
Development of in silico models of target receptors, identification of ‘hot-spots’ and molecular backbones of interest to be investigated, virtual screenings and selection of promising pharmaceutical candidates to be synthesised and optimized. The computational chemistry and drug design expertise of our scientific director Prof. Gabriele Cruciani and of the R&D group guide the development of this goal.

**Technical Highlights:**
• Design, optimization and use of software for the virtual screening of biological targets and ligands
• Target and ligand interactions simulation
• Physical-chemical properties predictions of drug candidates