D2 MEDICINAL CHEMISTRY GROUP – DRUG DISCOVERY MEDICINAL CHEMISTRY GROUP

Università Degli Studi di Perugia

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Área: Ciências Exatas
Linhas de Pesquisa: Antivirals; Antibacterials; Anticancer

Breve descrição das atividades de pesquisa

D2 Medicinal Chemistry Group has significant expertise in the field of medicinal chemistry and drug discovery. The members are involved on the design, synthesis and discovery of new chemical entities with defined biological activity. In particular, the research activities mainly concern the application/development of advanced methodologies of molecular modeling, chemoinformatics and library design in order to: 1) study the structure function relationships of macromolecules of biological interest; 2) identify and optimize new bioactive compounds through rational ligand- and target-based design, characterization of structure-activity relationships as well as virtual screening; 3) understand the factors determining the binding of a ligand to the biological target, 5) predict the physico-chemical properties and pharmacokinetics of compounds of pharmaceutical interest. Research is focused on the identification and optimization of new hit/lead compounds. The main skills are: (i) rational design of new compounds also through the use of basic computational methods, (ii) planning and optimization of synthetic routes, including the use of the microwave synthesis and parallel synthesis, for the preparation of new chemical entities, (iii) chemical characterization of the synthesized compounds by instrumental techniques such as NMR, IR, UV, HRMS and purification of the compounds through chromatographic separation methods, (iv) bibliographic study and selection of new "drugable targets" for innovative therapies.

Impacto das pesquisas desenvolvidas para a sociedade e ciência

Research projects are carried out in cooperation with research groups from all the world. Among the projects, the following can be highlighted: antimicrobial resistance (bacteria, mycobacteria, and fungi), viral infections (HCV, HIV, Influenza A, and flavivirus (e.g. Dengue)), cancer (miRNA regulation and PARP proteins), neurodegenerative diseases (Alzheimer’s disease, Huntington’s disease, Multiple sclerosis, and Prion diseases), and Inflammation (protein kinases).

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