



DRUG DESIGN AND DISCOVERY

DEPARTMENT OF PHARMACEUTICAL CHEMISTRY

ABOUT THE GROUP

The design and discovery of new neuroprotective and anti-neoplastic drugs combines advanced computational and chemical methods. Research into the mechanisms of neurological and cancer diseases reveals drug targets – epigenetic proteins, GPCRs and protein kinases – whose modulation delivers better efficacy in modern therapy.

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MAIN RESEARCH FOCUS

- Drug design & discovery of neuroprotective and antineoplastic drugs
- Pharmacophore modeling, 3D-QSAR & virtual screening
- Molecular docking & molecular dynamics simulations
- Computer-aided drug design & biopharmaceutical profiling



PROJECTS

- **Novel DOT1L and DNMT1/3A inhibitors** Pavle Savić **bilateral** France–Serbia · Institut Pasteur/CNRS, Paris · 2020–2022
- **Light-triggered control of epigenetic states** DFG project · Philipps-Universität Marburg · 2020–2023
- **COST Actions – CA20113 and CA21135 (IMMUNO-model)** European research networks · 2019–2026



PARTNER INSTITUTIONS

Institut Pasteur / CNRS (FR) · University of Marburg (DE) · University of St Andrews & UEA (UK) · CSIC Madrid (ES) · University of Eastern Finland · VINČA Institute & IORS (RS)

KEYWORDS

Drug design

3D-QSAR

Virtual screening

CADD

Molecular docking

GPCRs

Epigenetics

AT A GLANCE



9 researchers



6 projects



10 collaborations



Full profile,
publications and
collaborations