

CCR – IMPROMPTU

Wednesday, April 29th 2026, 11:00 AM

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FROM ALGORITHMS TO THE BENCH: AI-POWERED DRUG DISCOVERY FOR HARD-TO-DRUG PROTEINS IN CANCER

Advances in artificial intelligence (AI) are beginning to transform early-stage drug discovery, particularly for protein targets long considered “undruggable.” In this talk, I will first summarize our recent Nature Biotechnology paper in which we developed and applied an AI- and quantum-enhanced generative framework to design and prioritize small-molecule inhibitors against challenging cancer-relevant targets such as KRAS, demonstrating that data-driven molecular generation can efficiently navigate vast chemical space and yield compounds with validated cellular activity. Building on this work, we are now deploying this integrated AI platform across dozens of hard-to-drug protein targets (predominantly small GTPases and RTKs) implicated in diverse cancers. A central component of our strategy is the tight coupling of in silico design with in-house developed live-cell technologies (MaMTH, SIMPL, and CLIP-LUX) which enable systematic characterization, validation, and functional profiling of small-molecule modulators directly in physiologically relevant cellular contexts. In the second part of the talk, I will present our recent discovery of a therapeutic vulnerability in glioblastoma uncovered using the Mammalian Membrane Two-Hybrid high-throughput (MaMTH-HTS) live-cell interaction platform, and discuss how such insights can open new avenues for intervention in glioblastoma, one of the most difficult-to-treat cancers. These studies illustrate how integrating AI with live-cell technologies developed in our lab enables both the discovery of new druggable targets and the identification of previously unknown players in difficult-to-treat cancers such as glioblastoma.

Venue: Lecture Hall B2, Borschkegasse 4a

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Host: Maria Sibilja



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