(Q)SAR Directed Design, Synthesis and Evaluation of Anti-Invasive Chalcones and Analogues

Bart I. Roman¹, Marc E. Bracke² Alan R. Katritzky³, and Christian V. Stevens¹

¹ Research Group SynBioC, Department of Sustainable Organic Chemistry and Technology, Faculty of Bioscience Engineering, Coupure Links 653, B-9000 Ghent, Belgium. E-mail address: bart1.roman@ugent.be; ² Laboratory of Experimental Cancer Research, Department of Radiation Oncology and Experimental Cancer Research, Ghent University Hospital, De Pintelaan 185, B-9000 Ghent, Belgium; ³ Center for Heterocyclic Compounds, Department of Chemistry, 127 Chemistry Research Building, University of Florida, Gainesville, FL32611-7200, United States of America.

The processes of invasion and metastasis account for 90% of human cancer fatalities. Since no efficient drugs tackling these phenomena are available in the clinic today, their development represents a cardinal challenge in contemporary cancer research.

We have embarked on a QSAR-directed search for potent anti-invasive compounds, starting from natural chalcones. Via an in vitro feedback loop, we were able to identify several interesting lead candidates. Furthermore, one compound was taken to the in vivo level and showed promising behavior in a xenograft model in nude mice.