CORE

(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: <u>bart1.roman@ugent.be</u>;
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.

