Accepted Manuscript

Discovery of 4-[(5-arylidene-4-oxothiazolidin-3-yl)methyl]benzoic acid derivatives active as novel potent allosteric inhibitors of protein tyrosine phosphatase 1B: In silico studies and in vitro evaluation as insulinomimetic and anti-inflammatory agents

Rosaria Ottanà, Paolo Paoli, Alexandra Naß, Giulia Lori, Venera Cardile, Ilenia Adornato, Archimede Rotondo, Adriana Carol Eleonora Graziano, Gerhard Wolber, Rosanna Maccari

PII: S0223-5234(16)30934-5

DOI: 10.1016/j.ejmech.2016.10.063

Reference: EJMECH 9028

To appear in: *European Journal of Medicinal Chemistry*

Received Date: 23 July 2016

Revised Date: 26 September 2016

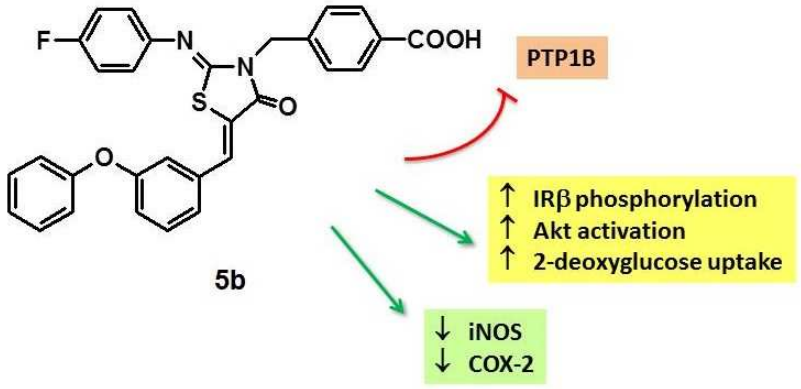
Accepted Date: 30 October 2016

Please cite this article as: R. Ottanà, P. Paoli, A. Naß, G. Lori, V. Cardile, I. Adornato, A. Rotondo, A.C. Eleonora Graziano, G. Wolber, R. Maccari, Discovery of 4-[(5-arylidene-4-oxothiazolidin-3-yl)methyl]benzoic acid derivatives active as novel potent allosteric inhibitors of protein tyrosine phosphatase 1B: In silico studies and in vitro evaluation as insulinomimetic and anti-inflammatory agents, *European Journal of Medicinal Chemistry* (2016), doi: 10.1016/j.ejmech.2016.10.063.

Graphical abstract

Discovery of 4-[(5-arylidene-4-oxothiazolidin-3-yl)methyl]benzoic acid derivatives active as novel potent allosteric inhibitors of protein tyrosine phosphatase 1B: In silico studies and in vitro evaluation as insulinomimetic and anti-inflammatory agents

Rosaria Ottanà, Paolo Paoli, Alexandra Naß, Giulia Lori, Venera Cardile, Ilenia Adornato, Archimede Rotondo, Adriana Carol Eleonora Graziano, Gerhard Wolber, Rosanna Maccari



In silico studies and biological evaluation of new 4-thiazolidinone derivatives, which were designed and synthesised as inhibitors of protein tyrosine phosphatase 1B, led to the identification of novel potent allosteric inhibitors of the target enzyme as well as to a new lead compound (**5b**) endowed with promising insulinomimetic and anti-inflammatory properties in cell-based models.