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Abstract

Pyridazin-3(2H)-one as New FABP4 Inhibitors Suggested by Molecular Growing Experiments †

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Abstract: The therapeutic potential of fatty acid binding protein 4 (FABP4) is widely acknowledged. Currently, there are numerous clinical studies that indicate how fatty acid binding protein 4 inhibitors could be useful in the treatment of various diseases. To identify new and more potent inhibitors, we utilized a two-step computational approach to design novel structures. Through the use of this approach, we were able to identify a new class of FABP4 inhibitors (FABP4i IC50 2.97 to 23.18 μM) that are capable of inhibiting the activity of FABP4 as low as Arachidonic acid (FABP4i IC50 3.42 ± 0.54 μM). In this study, we present the detailed structural and biological evaluation, and the synthetic procedures of the new pyridazinone-based scaffold FABP4i.

Keywords: fatty acid binding protein; FABP4; FABP4is; FABP4 inhibitors; pyridazinone; computing assisted molecular design

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