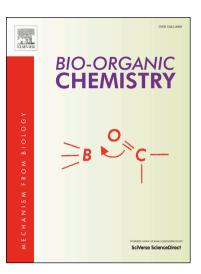
Accepted Manuscript

Design, synthesis and molecular docking of thiazolidinedione based benzene sulphonamide derivatives containing pyrazole core as potential anti-diabetic agents

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PII:	S0045-2068(17)30664-8
DOI:	https://doi.org/10.1016/j.bioorg.2017.11.010
Reference:	YBIOO 2170
To appear in:	Bioorganic Chemistry
Received Date:	30 August 2017
Revised Date:	14 November 2017
Accepted Date:	15 November 2017



Please cite this article as: Mohd. Javed Naim, O. Alam, Md. Jahangir Alam, Md. Quamrul Hassan, N. Siddiqui, V.G.M. Naidu, Md. Iqbal Alam, Design, synthesis and molecular docking of thiazolidinedione based benzene sulphonamide derivatives containing pyrazole core as potential anti-diabetic agents, *Bioorganic Chemistry* (2017), doi: https://doi.org/10.1016/j.bioorg.2017.11.010

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ACCEPTED MANUSCRIPT

Design, synthesis and molecular docking of thiazolidinedione based benzene sulphonamide derivatives containing pyrazole core as potential anti-diabetic agents Mohd. Javed Naim¹, Ozair Alam¹*, Md. Jahangir Alam¹, Md. Quamrul Hassan², Nadeem

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Abstract

We herein report the design, synthesis and molecular docking studies of 2,4-thiazolidinedione derivatives containing benzene sulphonyl group which are docked against the Peroxisome Proliferator Activated Receptor (PPAR γ) target. Compound **7p** was most effective in lowering the blood glucose level as compared to standard drugs pioglitazone and rosiglitazone. Compound **7p** exhibited potent PPAR- γ transactivation of 61.2% with 1.9 folds increase in gene expression. In molecular docking studies **7p** showed excellent interactions with amino acids **TYR** 473, SER 289, HIE 449, **TYR** 327, ARG 288, MET 329 and LEU 228. Compound **7p** did not cause any damage to the liver without any noteworthy weight gain and may be considered as promising candidates for the development of new antidiabetic agents.

Keywords: Anti-diabetic; PPAR γ ; Gene expression; Molecular docking; Thiazolidinedione; Pyrazole.

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