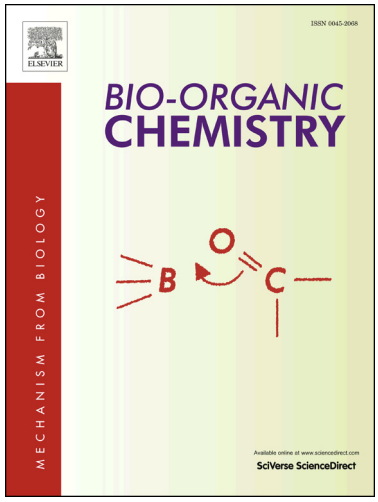

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Synthesis and *In Silico* Studies of Novel Sulfonamides having Oxadiazole Ring: As *β*-Glucuronidase Inhibitors

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Abstract

Novel sulfonamides having oxadiazole ring were synthesized by multistep reaction and evaluated to check *in vitro β*-glucuronidase inhibitory activity. Luckily, except compound **13**, all compounds were found to demonstrate good inhibitory activity in the range of IC_{50} = 2.40 ± 0.01-58.06 ± 1.60 μM when compared to the standard D-saccharic acid 1,4-lactone (IC_{50} = 48.4 ± 1.25 μM). Structure activity relationship was also presented. However, in order to ensure the SAR as well as the molecular interactions of compounds with the active site of enzyme, molecular docking studies on most active compounds **19**, **16**, **4** and **6** was carried out. All derivatives were fully characterized by ^{1}H-NMR, ^{13}C-NMR and EI-MS spectroscopic techniques. CHN analysis was also presented.

Keywords: Synthesis, Oxadiazole, Sulfonamides, *In Vitro*, *β*-Glucuronidase Inhibitory Activity, *In Silico*

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