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New potent STS inhibitors based on fluorinated 4-(1-phenyl-1*H*-[1,2,3]triazol-4-yl)-phenyl sulfamates

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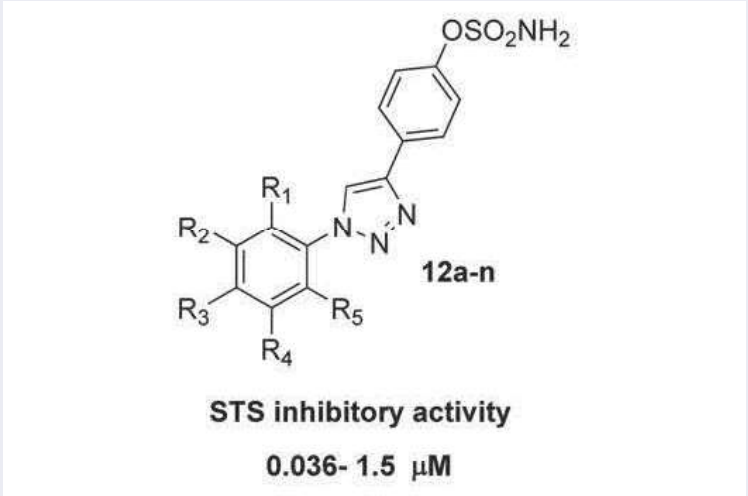
ABSTRACT

A series of fluorinated analogs based on the frameworks of 4-(1-phenyl-1*H*-[1,2,3]triazol-4-yl)-phenyl sulfamates have been synthesized as steroid sulfatase (STS) inhibitors. The design of chemical structures of new potential STS inhibitors was supported by molecular docking techniques to identify potential interactions between inhibitors and amino acid residues located in the STS active site. The STS inhibitory potency was evaluated on STS isolated from human placenta. We found that compounds substituted with fluorine atom at the *meta* position demonstrated the highest inhibitory effects in enzymatic STS assay. The most active analog **12e** – inhibited STS enzyme with the IC_{50} value of 36 nM.



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