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Pharmacophore modeling for discovery of 6,7-Dihydro-5H-pyrrolo[2,3-a]pyrimidines as orally available G Protein-Coupled Receptor 119 agonists

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Abstract: In the present work, pharmacophore modeling for discovery of 6,7-Dihydro-5H-pyrrolo[2,3-a]pyrimidines as orally available G Protein-Coupled Receptor 119 agonists has been performed to understand the pharmacophoric features. The analysis involves the comparison of pharmacophore model of most and least active molecules of the series. The analysis is successful in instituting the structure-activity relationships.

Introduction: Type-2 diabetes is a disease characterized by hyperglycemia, insulin resistance, and deficiency of insulin secretion from pancreatic β-cells. Glycemic regulation is very important for metabolic homeostasis, generally, uninhibited hyperglycemia leads to long-term complications comprising organ failure and amputation. Recent studies indicate that GPR119 has key role in glucosehomeostasis [1]. Specially, GPR119 agonists have been revealed tocause nutrient-independent incretion and GI hormone release aswell as nutrient-stimulated insulin secretion,thus, pulling down plasma glucose levels during an oral glucose tolerancetest [1]. Recently, 6,7-Dihydro-5H-pyrrolo[2,3-a]pyrimidines were synthesized and assayed for G Protein-Coupled Receptor (GPCR) 119 agonists. Pharmacophore modeling is a thriving branch of modern drug designing, which has been used frequently for drug and lead optimization. In the present work, pharmacophore modeling was performed for discovery of 6,7-Dihydro-5H-pyrrolo[2,3-a]pyrimidines as orally available G Protein-Coupled Receptor 119 agonists.

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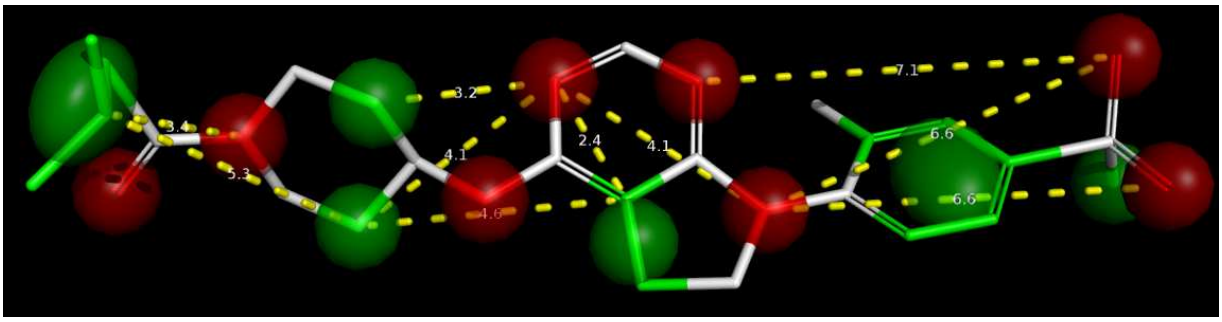

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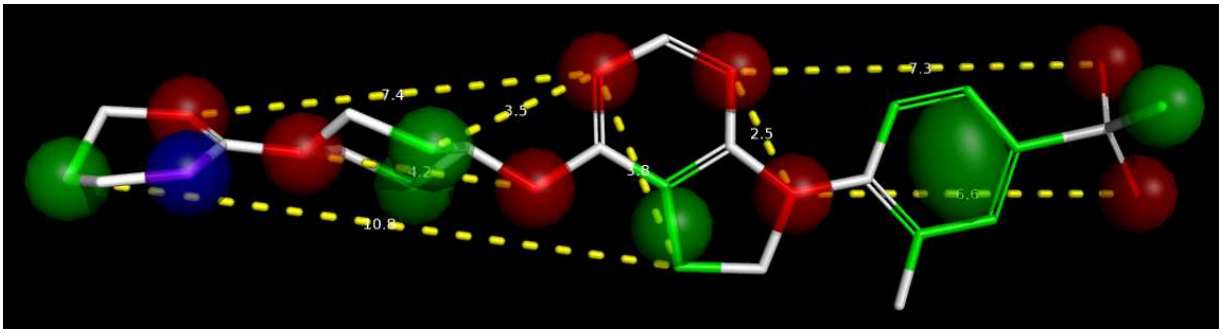

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