

# Medicinal Chemistry & Computer Aided Drug Designing

November 02-04, 2015 Atlanta, USA

## Computational studies of dipeptidyl peptidase IV inhibitors

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Diabetes is an illness characterized by abnormally high level of glucose in blood. Type 2 diabetes (T2D) is one of the major concerns for the health of individual around the World in 21st century as the prevalence of diabetes is increased apace. Dipeptidyl Peptidase IV (DPP IV) inhibitors are relatively new therapy for management of T2D. Inhibition of DPP-IV is an attractive new approach to the management of type 2 diabetes. DPP IV belongs to a family of prolyl-specific proteases that consists of several closely related enzymes in family: DPP-2/QPP, DPP-8, DPP-9, FAP- $\alpha$ . DPP IV is a highly specific serine aminoprotease that preferentially cleaves oligopeptides. It cleaves peptide from N-terminal where penultimate (P1) amino acid is either alanine or proline. X-ray crystal structure of DPP IV is solved in naïve form and inhibitor bound form. Around 85 solved crystal structures have been deposited to Protein Data Bank by different research groups till date. DPP IV inhibitors reported till date are chemically very diverse indicating that they may bind differently to active site of DPP IV. To understand binding mode of DPP IV inhibitors, diverse inhibitors were docked into active site of DPP IV. Result of the study revealed that vildagliptin and saxagliptin bind to unprimed S1 and S2 subsite of enzyme active site. Sitagliptin, teneligliptin, omarigliptin, carmegliptin, gosogliptin and anagliptin binds to S2 extensive site in addition to S1 and S2 subsite. Alogliptin and imigliptin binds to primed S1' site in addition to S1 and S2 subsite. Linagliptin occupies S1', S2' as well as S1 and S2 subsites. DPP IV inhibition tends to increase with increase in number of binding sites. All DPP IV inhibitors make important hydrophobic interaction with S1 subsite and salt bridge interactions with GLU205 and/ or GLU206 motif.

### Biography

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