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Development of QAAR models to explore the selectivity profile of PPAR α , δ and γ modulators

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Disease related to metabolic syndrome is an interesting topic to the researchers throughout the world. The peroxisome proliferator-activated receptors (PPAR α , δ , and γ) are the members of the nuclear receptor family, which play important roles in regulation of metabolism, inflammation, and cell differentiation, it is seemed to be very much related with metabolic syndrome. These receptor subtypes are very much interrelated on the basis of their homology and the active catalytic sides. In the present approach, quantitative activity-activity relationship (QAAR) has been performed to develop the relationship between selectivity of modulators of each subtypes over others. It is observed that there is a positive influence of γ and δ subtypes modulators, whereas α and δ subtypes modulators have a negative influence on each other. Similarly, it is also seen that the descriptor contribution is different for each subtypes. For the γ and δ selectivity, the descriptors- electrotopological state keys (JX), atom type indices (Atype_O_59), jurs (Jurs-RPCG) and atom pairs indices T(S..F) have opposite contribution to develop the QAAR model. But for the α subtype modulation, different type descriptors, such as ETA descriptor (ETA_Shape_X), constitutional indices (nAB), functional group counts (nCONHRPh and nHDOn), and atom type indices (Atype_F_84, Atype_N_71 and Atype_C_34) show the importance of selectivity contribution.

Biography

Achintya Saha, Professor and Head, Department of Chemical Technology, University of Calcutta, India has 20 years teaching and research experience in Pharmaceutical fields, especially in Drug Design through Cheminformatics techniques. He completed his PhD in Pharmaceutical Technology from Jadavpur University, India and did Post-doctoral research in University of North Carolina, USA. He has published more than 100 papers in peer reviewed journals.

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