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Discovery of new microglial cathepsin S inhibitors for the treatment of neuropathic pain: Pharmacophore modeling, 3D-QSAR and high-throughput screening

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Neuropathic pain occurs as a result of trauma or injury to a peripheral nerve due to damage or dysfunction of the nervous system under various disease conditions. Lysosomal Cysteine protease cathepsin S (CatS) plays a crucial role for the maintenance of neuropathic pain and spinal microglia activation. Thus, effective CatS inhibitors may be of significant therapeutic importance. In this study, a 3D pharmacophore mapping studies were undertaken for different series of synthetic derivatives. A five point pharmacophore with three hydrogen bond acceptors (A) one hydrogen bond donor (D), and one hydrophobic feature (H) as pharmacophoric features were developed. The pharmacophore hypothesis was validated with enrichment calculation best pharmacophore further yielded a statistically significant 3D-QSAR model, with a correlation coefficient of $R^2 = 0.992$ for training set compounds. The model generated showed excellent predictive power, with a correlation coefficient of $Q^2 = 0.7$. The model was then employed as 3D search query to screen against public and private compound libraries (Asinex, BITS database) in-order to identify a new scaffold. Best hit compounds were selected from virtual screening for the enzyme inhibitory In-vitro activity against CatS enzyme. Inhibitors IC50 value below 50μM were considered as potential selective non-peptidic and non-covalent inhibitors for CatS. Backbone structural scaffold features and the contour maps delivered from the built 3D QSAR models could serve as building blocks in designing novel drug molecules for CatS.

Biography

Madhu Babu Battu has completed his M.S (Pharm) from National Institute of Pharmaceutical Education and Research (NIPER), Hajipur. Currently, he is pursuing PhD from Pharmacy department at Birla Institute of Technology and Sciences (BITS-Pilani), Hyderabad campus, Jawaharnagar, Hyderabad. He has awarded CSIR-Senior Research Fellow from HRDG-CSIR, New Delhi in February 2012.

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The need of hexavalent vaccine: Future perspectives

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Hexavalent vaccines including Tetanus, Diphtheria, Pertussis, Hepatitis B, Polio and Haemophilus influenza type B antigens stand for the recent advance in the development of combination vaccines. DTP-Hep, Hib, IPV based combination vaccines formulation are now widely accepted as an effective means of eliciting protection against respective diseases. To meet societies increasing demands, global disease pressure, the DTP-Hep, Hib and IPV based combination vaccine production is highly required which is currently slow and meticulous- needs to embrace innovation to become significantly more cost effective that make more vaccine coverage. For this to happen, manufacturers urgently need new technological approaches that can rapidly and safely incorporate scientific discovery into scalable, adaptive vaccine manufacturing processes.

Here we provide an overview of innovative vaccine development technologies designed to produce hexavalent combination vaccine. In addition technological trends to solve the various issues regarding antigen selection (i.e Whole cell pertussis or acellular pertussis), adjuvant compatibility issues (Hib PRP with aluminum adjuvant) and preservative selection (thimersal or 2-Phenoxy Ethanol) in vaccines are discussed. Finally, we overviewed the need of hexavalent vaccine for global polio eradication and industry perspective.

The report concludes that there are silent new opportunities for overcoming bottlenecks and constraints within the existing vaccine production system through imaginative cross-disciplinary solutions and that need to be more focused, co ordinate domestic and international effort can accelerate progress toward more rapid production of safe, effective, affordable hexavalent pediatric combination vaccines.

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