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Designing de novo sequences of heparan sulfate that exhibit high selectivity for their target

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Designing glycosaminoglycan (GAG) sequences that target specific proteins is challenging and not yet achieved. This is a key reason that nature's library of millions of glycosaminoglycans (GAGs) sequences remains largely untapped. We have developed a very generalizable genetic algorithm-based dual-filter screening strategy that addresses this key hurdle. Our computational algorithm utilizes 'affinity' and 'specificity' filters and a combinatorial library of 46,656 heparan sulfate (HS) hexasaccharides binding to target protein(s) for identifying 'highly specific' HS sequences. Synthesis of these sequences followed by biochemical and biophysical studies help test the computational design predictions. This talk will focus on differential targeting of two highly similar proteins and will present design protocol for discovering high specificity GAG sequences. Considering that GAGs bind to several hundred human proteins, majority of which remain un-characterized with regard to GAG interactions, this work lays the pathway for discovering highly selective GAGs as drugs and/or chemical biology tools.

Biography

Umesh R Desai is the Director of Institute for Structural Biology, Drug Discovery and Development at Virginia Commonwealth University. He earned his PhD from Indian Institute of Technology, Bombay and did his Post-doctoral studies at Iowa, MIT and Illinois. He was awarded the Established Investigator Award by the American Heart Association and the Distinguished Scholarship Award by Virginia Commonwealth University.

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Page 50