Peptides play a significant role in the biological world. Optimization of peptide activity for a specific therapeutic target is a daunting task; owing to time and cost factor involved in the process. Specific computational approaches can simplify the task to elucidate the structural basis in the design of new peptides. Peptide QSAR approaches highlighted here being with simple Classical Hansch and Free-Wilson QSAR technique based models that make use of the amino acid properties (literature compiled or calculated theoretically) as X-variables to correlate the biological activity. The mathematical models so developed can explain and predict the position-wise specific nature and type of amino acids for a given peptide sequence. Uncertainties associated with the 3D-alignment of peptides in 3D-QSAR can be reduced by an approach coined as HomoSAR. The concept is centered on the homology modelling principles to result in 1D-alignment of the peptides though a multiple sequence alignment; followed by computation of position-wise similarity indices for amino acids in the peptide sequences. The third peptide QSAR approach referred to as ensemble QSAR (eQSAR) addresses the conformational ensemble issue as an improvement to the classical ‘one chemical–one structure–one parameter value’ dogma. The X-variables are calculated for the conformational ensemble for all peptides generated through molecular dynamic simulations. These descriptors (PD-Eigen values) are computed over Physicochemical Distance matrices (PD-matrices) that are unique to every conformation of every peptide; subsequently correlated to the biological activities. All the approaches have been tested on peptide datasets to put forth statistically validated QSAR models.

Biography
Raghuvir R S Pissurlenkar has completed his PhD (Tech) from Bombay College of Pharmacy, Mumbai University in Pharmaceutical Chemistry. He has worked at Bombay College of Pharmacy as an Assistant Professor of Pharmaceutical Chemistry from January 2006 till September 2014. At present he is an Associate Professor, Pharmaceutical Chemistry at Goa College of Pharmacy, Panaji Goa. His areas of research include Structure-based Ligand Design, Protein Modeling and Bio-molecular Simulations. He has 2 patents, 28 international and 4 national papers to his credit.

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