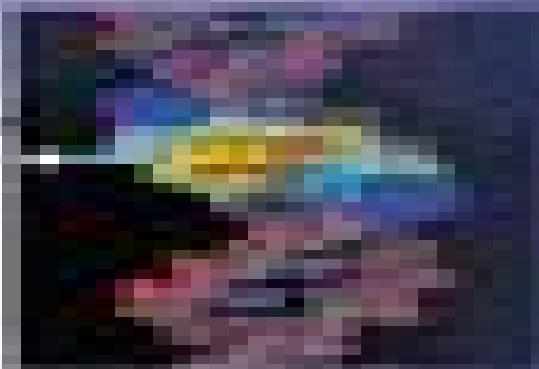
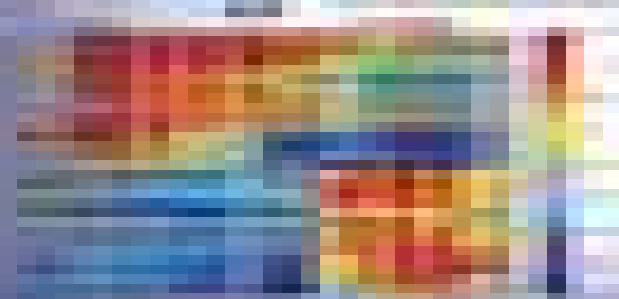


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Cheminformatics and Bioinformatics at the Interface with Systems Biology Aman Chandra Kaushik, Aamir Mehmood, Dong-Qing Wei, Sadia Nawab, Shakti Sahi, Ajay Kumar, 2023-09-08 The cost of drug development is increasing and investment returns are decreasing The number of drugs approved by FDA is in decline in terms of the number of new molecular entities NMEs Amongst the reasons noted for this are the adverse side effects and reduced efficiency of many of the potential compounds This is a problem both for the pharmaceutical industry and for those suffering from diseases for which there are no or few available treatments Advances in computational chemistry computer science structural biology and molecular biology have all contributed to improved drug design strategies and reduced the time taken for drug discovery By interfacing cheminformatics and bioinformatics with systems biology we can create a powerful tool for understanding the mechanisms of patho physiological systems and identifying lead molecules for various diseases This integration of drug design approaches can also play a crucial role in the prediction and rationalization of drug

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