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AI in Computational Drug Discovery

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Abstract

Ordinary medication revelation strategies depend essentially in-vitro tries directed with an objective particle and an extremely huge arrangement of little atoms to pick a correct ligand. With the investigation space for the correct ligand being exceptionally huge, this methodology is profoundly tedious and requires high capital for assistance. Virtual screening, a computational method utilized for assessing an enormous gathering of particles to recognize lead atoms, can be utilized for this reason to accelerate the medication revelation measure. Ligand based medication configuration works by building an applied model of the objective protein. Ligand based virtual screening utilizes this model to assess and isolate dynamic particles for an objective protein. A classes of calculation in machine inclining called Classification calculation can be utilized to construct the above model. In this theoretical, 3 distinctive AI ways to deal with settle virtual screening is depicted. The principal strategy uses a proficient virtual screening method utilizing Random Forest (RF) classifier. Second procedure applies SVM classifier for virtual screening. The third technique shows the appropriateness of Self Organizing Map (SOM) as a classifier for screening ligand atoms, which is first of its sort around there according to the writing. The discussion end with looking at the in addition to and short of the three strategies. The GPU parallelization of these techniques will be additionally clarified in subtleties

Biography:

He received his Ph.D in Computer Science from National Institute of Technology Calicut, India. His thesis was "GPU based Virtual Screening Techniques for Faster Drug Discovery". Now he is an assistant professor at the CSE department, NIT Calicut, India. His research interests include Medical-informatics, Computational Drug Design and GPU Computing. He has published many journals as well as conference proceedings. He has attended an International spring school on High Performance Computing (HighPer 2018) at San Sebastian, Spain in April 2018.

Speaker Publications:

1. "P. B. Jayaraj et al. Ligand based Virtual Screening using SVM on GPU, Computational Biology and Chemistry
2. "P. B. Jayaraj et al., GPURFSCREEN: A GPU based virtual screening tool using Random Forest Classifier, Journal of Cheminformatics.
3. Jayaraj, P. B et al., "A GPU based maximum common subgraph algorithm for drug discovery applications." In IPDPS Workshops, 580-588., Chicago,USA..

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