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Computational sciences span a broad range of research in computer-aided drug discovery and informatics. Computer-aided drug discovery investigates the relationships between ligands and their targets, using advanced statistical and rigorous thermodynamic methods. Simulations bridge the gap between the microscopic molecular and macroscopic whole animal “worlds”. Informatics approaches interrogate and investigate critical changes in the pathways in normal and disease-related biology. Novel methods are being developed to analyse massive amounts of experimental data, to isolate the key signals and induce interpretable hypotheses.

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