

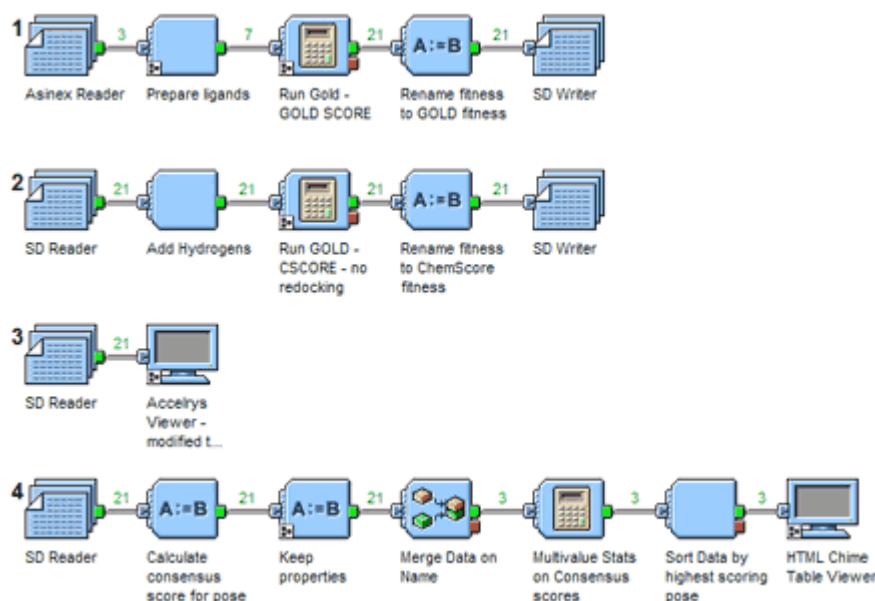


Virtual Screening using SciTegic Pipeline Pilot

Virtual Screening is the process of applying a computational model to a set of virtual or real molecules proposed for submission to screening, in order to select a subset for testing. This subset may be designed to minimize the number to test to identify the active information (minimize the false positives), to minimize the number of actives that will be missed (false negatives) or trade-off between the two.

A variety of virtual screening methods have been applied ranging and the method most appropriate depends on the quality and quantity of information available. If the receptor structure is known, then structure-based docking and scoring may be used. When only ligand activity is known, 3D modeling methods such as pharmacophore modeling may be used, or a variety of statistical methods using 2D or 3D descriptors may be applied.

Pipeline Pilot has application in each of these processes. For structure-based design and pharmacophore screening, it provides an automation platform to increase the efficiency of the process. For statistical modeling, it not only automates the process but provide the scientific methods to build models within its component collections.



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