A Linux based HTS data handling system

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Abstract: A high throughput screening (HTS) data handling system with a Web-based easy-to-use interface and corresponding databases has been developed. The constructed system incorporates all chemical, numerical and textual data related to the chemical compounds, assay plates, and the HTS assay itself and able to visualize the results using user friendly ways (IC_{50} graphs, colour coded plate-shaped graphs). The chemical type data (structure, mw, etc.) comes directly from our chemical and biological database. Users can search the database by traditional textual/numerical and/or chemical substructure or chemical similarity queries through the web interface. To build up our HTS data handling system, existing IT components such as ORACLE and SYBYL from Tripos for database management, and newly developed codes such as the Perl-cgi application frame and the Tcl/Tk data loader program was used. Linux was chosen as the main platform, however almost every component could be used under various operating systems.