Chemoinformatics in the Hit Triage Process:
Development of a Reporting System

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Subsequent to primary screening (or even before during library selection) one can be inundated by the number of active compounds. Implementation of chemoinformatics can reduce the number of compounds entering the more time and resource consuming hit follow-up process. The goal of our hit triage process is to identify and prioritise the most appropriate hit series following HTS. We have developed a tool to cluster actives, calculate physical properties and visualise output. Displayed information can be divided into molecular properties, rule filters, structural warnings and biological information and in order to optimise the decision making process the report is fully navigable. The report is implemented within SciTegic's Pipeline Pilot using CDK (Chemistry Development Kit) [1,2] for some chemoinformatic calculations.

[1] Steinbeck, C, Han, Y, Kuhn, S, Horlacher, O, Luttmann, E, and Willighagen, E. The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics, Journal of Chemical Information and Computer Sciences 43:493-500, 2003.

[2] Steinbeck, C, Hoppe, C, Kuhn, S, Floris, M, Guha, R, and Willighagen, E. Recent Developments of the Chemistry Development Kit (CDK) – An Open-Source Java Library for Chemo- and Bioinformatics, Current Pharmaceutical Design, 12, 2006, *in press*.