

A Pathvisio plugin for visualization of metabolite information

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ABSTRACT

Motivation: Recent developments have shown the importance of metabolomics in human systems biology research. Given their crucial and central role as particles capturing information from all functional levels of the cell, they can provide the link between transcription and actual phenotyping.(blog references) It is therefore important to develop tools that implement metabolomics data into for example pathway development tools such as Pathvisio. Pathvisio is an open source pathway development program that utilizes pathways in the WikiPathways database.(pathvisio reference) A high number of these pathways contain metabolites that play a crucial role in that pathway. The plugin for metabolite information can be used to access data for these metabolites directly from within the program without using a browser. The plugin visualizes widely used IDs, molecular formula's, SMILES, InChIs and implements NMR and MS data.

Results: Use-case: When selecting a metabolite in pathvisio, the plugin will show a number of types of data, including predicted Mass spectrometry and Nuclear Magnetic Resonance data.

Availability: The plugin is available on the plugin page of the Pathvisio website

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1 INTRODUCTION

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2 APPROACH

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3 METHODS

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[illegible]

*to whom correspondence should be addressed

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Fig. 2. Caption, caption.

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