

RetroPath2.0 parameters for Violacein

Below are listed the RetroPath2.0 parameters in order to reproduce the violacein results. See “*RetroPath2.0_tutorial*” file for a step-by-step guide.

Context

The violacein pathway consists of five pathway genes culminating in the production of violacein (and deoxyviolacein, due to promiscuity of the VioC enzyme,) and several additional intermediate and side products proceeding through spontaneous or unknown aerobic reactions.

Violacein is produced through a 5-step enzymatic process followed by a single non-enzymatic step.

Parameters

- Input
 - Pathway length: 5
 - Source: path to “*violacein/source.csv*” file (violacein and deoxyviolacein)
 - Sink: path to “*violacein/sink_A.csv*” file (all *E. coli* compounds)
 - Rules: path to “*violacein/rules.csv*” file (see **Rules** section)
- Output
 - Result folder: path to the desired output folder (should exist before execution)
- Result expected
 - The generated metabolic graph (*.json* file in the result folder) can be visualized using the Scope Viewer.

Rules

Rules have been selected according references. Below enzymes, EC numbers and associated MNXR IDs for each step:

- Enzyme: VioA
 - EC number(s): 1.4.3.-
 - MetaNetX reactions: MNXR2613, MNXR76570
- Enzyme: VioB

- EC number(s): 1.21.98.-
 - MetaNetX reactions: MNXR85789
- Enzyme: VioE
 - MetaNetX reactions: MNXR87814
- Enzyme: VioD
 - EC number(s): 1.14.13.217
 - MetaNetX reactions: MNXR62938
- Enzyme: VioC
 - EC number(s): 1.14.13.224
 - MetaNetX reactions: MNXR62939, MNXR62941
- Spontaneous
 - MetaNetX reactions: MNXR62940, MNXR62942, MNXR62943, MNXR62944

References

- PMID: 26062452
- PMID: 21779844
- MetaCyc Pathway ID: PWY-7040