RetroPath2.0 parameters for Carotene

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

Parameters

- Input

  - Pathway length: 5
  - Source: path to *"carotene/source.csv"* file (beta-carotene)
  - Sink: path to *"carotene/sink.csv"* file (all *E. coli* compounds)
  - Rules: path to *"carotene/rules.csv"* file (see **Rules** section)

- Output

  - Result folder: path to the desired output folder (should exists 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 to references. Below enzymes, EC numbers and associated MNXR IDs for each step:

- Enzyme: GGPP synthase

  - EC number(s): 2.5.1.29
  - MetaNetX reactions: MNXR55435

- Enzyme: phytoene synthase

  - EC number(s): 2.5.1.32
  - MetaNetX reactions: MNXR71200, MNXR70495, MNXR15602, MNXR8603, MNXR87812, MNXR67228

- Enzyme: phytoene desaturase

  - EC number(s): 1.3.99.31, 1.3.99.28
  - MetaNetX reactions: MNXR26357, MNXR26773, MNXR26774

- Enzyme: lycopene cyclase

  - EC number(s): 5.5.1.19
  - MetaNetX reactions: MNXR15454, MNXR16029, MNXR60336, MNXR17616, MNXR9555,

References:

- PMID: 25403509
- MetaCyc pathway ID: PWY-7393