RetroPath2.0 parameters for Pinocembrin

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

Case A

- Input

  – Pathway length: 4
  – Source: path to *"pinocembrin/source.csv"* file (pinocembrin)
  – Sink: path to *"pinocembrin/sink_A.csv"* file (phenylalanine)
  – Rules: path to *"pinocembrin/rules.csv"* file (see **Rules** section)

- Output

  – Result folder: path to the desired output folder (should exists before execution)

- Result expected

  – No scope found since side-products of some reactions are not in sink.

Case B

- Input

  – Pathway length: 4
  – Source: path to *"pinocembrin/source.csv"* file (pinocembrin)
  – Sink: path to *"pinocembrin/sink_B.csv"* file (all *E. coli* compounds)
  – Rules: path to *"pinocembrin/rules.csv"* file

- 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 references. Below enzymes, EC numbers and associated MNXR IDs for each step:

- Enzyme: PAL

- EC number(s): 4.3.1.24, 4.3.1.25
  - MetaNetX reactions: MNXR7145, MNXR93681

- Enzyme: 4CL

  - EC number(s): 6.2.1.12
  - MetaNetX reactions: MNXR1041, MNXR2251, MNXR227, MNXR14993, MNXR60189

- Enzyme: CHS

  - EC number(s): 2.3.1.74
  - MetaNetX reactions: MNXR84871, MNXR85701, MNXR85702, MNXR27480

- Enzyme: CHI

  - EC number(s): 5.5.1.6
  - MetaNetX reactions: MNXR60602, MNXR70709, MNXR73989, MNXR84948, MNXR85459, MNXR85703, MNXR76242

References

- PMID: 25085569