

ABSTRACT

SYNTHETIC PATHWAY GENERATING APPARATUS, SYNTHESIS PATHWAY GENERATING METHOD, SYNTHESIS PATHWAY GENERATING PROGRAM, AND METHOD OF PRODUCING 3-HYDROXYPROPIONIC ACID, CROTONYL ALCOHOL AND BUTADIENE

A compound synthetic pathway is generated without limiting chemical conversion rules. A synthetic pathway generating apparatus includes: a converting unit to convert chemical structures of compounds into numerical values; a calculation unit to create a compound pair and to calculate a difference value by subtracting the numerical value of one compound of the compound pair from the numerical value of the other compound thereof; a determining unit to compare the difference value of the compound pair of the reaction between which is already known with the difference value of the compound pair of the reaction between which is unknown, and to determine unknown reactions of the compound pairs with the difference values being coincident as virtual reactions; a generating unit to generate compound synthetic pathways by use of nodes representing the compounds and edges representing the known reaction and the virtual reaction respectively; and a selecting unit to select a synthetic pathway from a starting compound to a target compound out of the generated compound synthetic pathways.

Figure 8