CLAIMS

1. A synthetic pathway generating apparatus comprising:

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 a compound pair of the reaction between which is already known with the difference value of a compound pair of the reaction between which is unknown, and to determine the unknown reaction of the compound pair with the difference value being coincident with the difference value of the known reaction as a virtual reaction;

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.

2. The synthetic pathway generating apparatus according to claim 1, comprising a thermodynamic determination unit to determine thermodynamic feasibility about the selected synthetic pathway.

3. The synthetic pathway generating apparatus according to claim 1 or 2, comprising a (molar) theoretical yield determining unit to calculate a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and to determine whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

4. A synthetic pathway generating apparatus comprising:

a converting unit to convert chemical structures of compounds into numerical values;

a first calculation unit to create a compound pair and to calculate a first difference value by subtracting the numerical value of one compound of the compound pair from the numerical value of the other compound thereof;

a second calculation unit to calculate a second difference value by subtracting the numerical value of a starting compound from the numerical value of a target compound; and

a generating unit to generate, by use of the starting compound, the target compound and the plurality of first difference values, a synthetic pathway wherein a total value of the first difference values in the synthetic pathway from the starting compound to the target compound is coincident with the second difference value.

5. The synthetic pathway generating apparatus according to claim 4, comprising a (molar) theoretical yield determining unit to calculate a (molar) theoretical yield of the target compound synthesized by the synthetic pathway and to determine whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

6. The synthetic pathway generating apparatus according to claim 5, comprising a thermodynamic determination unit to determine thermodynamic feasibility about the synthetic pathway.

7. A synthetic pathway generating method by which a computer executes:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating 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 step of comparing 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 determining the unknown reaction of the compound pair with the difference value being coincident with the difference value of the known reaction as a virtual reaction;

a step of generating compound synthetic pathways by use of nodes representing the compounds and edges representing the known reaction and the virtual reaction respectively; and

a step of selecting a synthetic pathway from a starting compound to a target compound out of the generated compound synthetic pathways.

8. The synthetic pathway generating method according to claim 7, wherein the computer executes a step of determining thermodynamic feasibility about the

selected synthetic pathway.

9. The synthetic pathway generating method according to claim 7 or 8, wherein the computer executes a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

10. A synthetic pathway generating method by which a computer executes:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating a first difference value by subtracting the numerical value of one compound of the compound pair from the numerical value of the other compound thereof;

a step of calculating a second difference value by subtracting the numerical value of a starting compound from the numerical value of a target compound; and

a step of generating, by use of the starting compound, the target compound and the plurality of first difference values, a synthetic pathway wherein a total value of the first difference values in the synthetic pathway from the starting compound to the target compound is coincident with the second difference value.

11. The synthetic pathway generating method according to claim 10, wherein the computer executes a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

12. The synthetic pathway generating method according to claim 11, wherein the computer executes a step of determining thermodynamic feasibility about the selected synthetic pathway.

13. A synthetic pathway generating program for making a computer execute:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating 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 step of comparing 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 determining the unknown reaction of the compound pair with the difference values being coincident with the difference value of the known reaction as a virtual reaction;

a step of generating compound synthetic pathways by use of nodes representing the compounds and edges representing the known reaction and the virtual reaction respectively; and

a step of selecting a synthetic pathway from a starting compound to a target compound out of the generated compound synthetic pathways.

14. The synthetic pathway generating program according to claim 13, for making the computer execute a step of determining thermodynamic feasibility about the selected synthetic pathway.

15. The synthetic pathway generating program according to claim 13 or 14, for making the computer execute a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

16. A synthetic pathway generating program for making a computer execute:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating a first difference value by subtracting the numerical value of one compound of the compound pair from the numerical value of the other compound thereof;

a step of calculating a second difference value by subtracting the numerical value of a starting compound from the numerical value of a target compound; and

a step of generating, by use of the starting compound, the target compound and the plurality of first difference values, a synthetic pathway wherein a total value of the first difference values in the synthetic pathway from the starting compound to the target compound is coincident with the second difference value.

17. The synthetic pathway generating program according to claim 16, for making the computer execute a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and

determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

18. The synthetic pathway generating program according to claim 17, for making the computer execute a step of determining thermodynamic feasibility about the selected synthetic pathway.

19. A method for producing 3-hydroxypropionic acid, comprising the step of reductively decarboxylating oxaloacetate to convert oxaloacetate into 3-hydroxypropionic acid.

20. A method for producing 3-hydroxypropionic acid, comprising culturing, in a medium containing a carbon source, a microorganism which has the ability to produce 3-hydroxypropionic acid and the enzyme activity to reductively decarboxylate oxaloacetate to convert oxaloacetate into 3-hydroxypropionic acid, thereby allowing to accumulate 3-hydroxypropionic acid in the medium or the cells; and collecting the 3-hydroxypropionic acid from the medium or the cells.

21. A method for producing 3-hydroxypropionic acid, comprising the step of reductively decarboxylating oxaloacetate to convert oxaloacetate into malonate; and the step of converting malonate into 3-hydroxypropionic acid.

22. A method for producing 3-hydroxypropionic acid, comprising culturing, in a medium containing a carbon source, a microorganism which has the ability to produce 3-hydroxypropionic acid, the enzyme activity to reductively decarboxylate oxaloacetate to convert oxaloacetate into malonate, and the enzyme activity to convert malonate into 3-hydroxypropionic acid, thereby allowing to accumulate 3-hydroxypropionic acid in the medium or the cells; and collecting the 3-hydroxypropionic acid from the medium or the cells.

23. A method for producing malonate, comprising the step of reductively decarboxylating oxaloacetate to convert oxaloacetate into malonate.

24. A method for producing 3-hydroxypropionic acid, comprising the step of decarboxylating pyruvate to convert pyruvate into formate; and the step of converting formate into 3-hydroxypropionic acid.

25. A method for producing 3-hydroxypropionic acid, comprising culturing, in a medium containing a carbon source, a microorganism which has the ability to produce 3-hydroxypropionic acid, the enzyme activity to decarboxylate pyruvate to convert pyruvate into formate, and the enzyme activity to convert formate into 3-hydroxypropionic acid, thereby allowing to accumulate 3-hydroxypropionic acid

in the medium or the cells; and collecting the 3-hydroxypropionic acid from the medium or the cells.

26. A method for producing formate, comprising the step of decarboxylating pyruvate to convert pyruvate into formate.

27. A method for producing 3-hydroxypropionic acid, comprising the step of converting C02107 ((*S*,*S*)-tartaric acid) into C00222 (3-oxopropanoate), and the step of converting C00222 into 3-hydroxypropionic acid.

28. A method for producing 3-hydroxypropionic acid, comprising culturing, in a medium containing a carbon source, a microorganism which has the ability to produce 3-hydroxypropionic acid, the enzyme activity to convert C02107 into C00222, and the enzyme activity to convert C00222 into 3-hydroxypropionic acid, thereby allowing to accumulate 3-hydroxypropionic acid in the medium or the cells; and collecting the 3-hydroxypropionic acid from the medium or the cells.

29. A method for producing C00222, comprising the step of converting C02107 into C00222.

30. A method for producing crotonyl alcohol, comprising the step of converting acetyl-CoA into acetoacetyl-CoA; the step of converting acetoacetyl-CoA into 3-hydroxybutyl-CoA; the step of converting 3-hydroxybutyl-CoA into crotonyl-CoA; the step of converting crotonyl-CoA into crotonyl aldehyde; and the step of converting crotonyl aldehyde into crotonyl alcohol.

31. A method for producing crotonyl alcohol, comprising culturing, in a medium containing a carbon source, a microorganism which has the ability to produce crotonyl alcohol, enzyme activity to convert acetyl-CoA into acetoacetyl-CoA, the enzyme activity to convert acetoacetyl-CoA into 3-hydroxybutyl-CoA, the enzyme activity to convert 3-hydroxybutyl-CoA into crotonyl-CoA, the enzyme activity to convert crotonyl-CoA into crotonyl aldehyde, and the enzyme activity to convert crotonyl aldehyde into crotonyl alcohol, thereby allowing to accumulate crotonyl alcohol in the medium or the cells; and collecting the crotonyl alcohol from the medium or the cells.

32. A method for producing butadiene, comprising producing crotonyl alcohol by the process according to claim 30 or 31; and dehydrating the resultant crotonyl alcohol to give butadiene.

CLAIMS

1. A synthetic pathway generating apparatus comprising:

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 a compound pair of the reaction between which is already known with the difference value of a compound pair of the reaction between which is unknown, and to determine the unknown reaction of the compound pair with the difference value being coincident with the difference value of the known reaction as a virtual reaction;

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.

2. The synthetic pathway generating apparatus according to claim 1, comprising a thermodynamic determination unit to determine thermodynamic feasibility about the selected synthetic pathway.

3. The synthetic pathway generating apparatus according to claim 1 or 2, comprising a (molar) theoretical yield determining unit to calculate a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and to determine whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

4. A synthetic pathway generating apparatus comprising:

a converting unit to convert chemical structures of compounds into numerical values;

a first calculation unit to create a compound pair and to calculate a first difference value by subtracting the numerical value of one compound of the compound pair from the numerical value of the other compound thereof;

a second calculation unit to calculate a second difference value by subtracting the numerical value of a starting compound from the numerical value of a target compound; and

a generating unit to generate, by use of the starting compound, the target compound and the plurality of first difference values, a synthetic pathway wherein a total value of the first difference values in the synthetic pathway from the starting compound to the target compound is coincident with the second difference value.

5. The synthetic pathway generating apparatus according to claim 4, comprising a (molar) theoretical yield determining unit to calculate a (molar) theoretical yield of the target compound synthesized by the synthetic pathway and to determine whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

6. The synthetic pathway generating apparatus according to claim 5, comprising a thermodynamic determination unit to determine thermodynamic feasibility about the synthetic pathway.

7. A synthetic pathway generating method by which a computer executes:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating 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 step of comparing 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 determining the unknown reaction of the compound pair with the difference value being coincident with the difference value of the known reaction as a virtual reaction;

a step of generating compound synthetic pathways by use of nodes representing the compounds and edges representing the known reaction and the virtual reaction respectively; and

a step of selecting a synthetic pathway from a starting compound to a target compound out of the generated compound synthetic pathways.

8. The synthetic pathway generating method according to claim 7, wherein the computer executes a step of determining thermodynamic feasibility about the

selected synthetic pathway.

9. The synthetic pathway generating method according to claim 7 or 8, wherein the computer executes a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

10. A synthetic pathway generating method by which a computer executes:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating a first difference value by subtracting the numerical value of one compound of the compound pair from the numerical value of the other compound thereof;

a step of calculating a second difference value by subtracting the numerical value of a starting compound from the numerical value of a target compound; and

a step of generating, by use of the starting compound, the target compound and the plurality of first difference values, a synthetic pathway wherein a total value of the first difference values in the synthetic pathway from the starting compound to the target compound is coincident with the second difference value.

11. The synthetic pathway generating method according to claim 10, wherein the computer executes a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

12. The synthetic pathway generating method according to claim 11, wherein the computer executes a step of determining thermodynamic feasibility about the selected synthetic pathway.

13. A synthetic pathway generating program for making a computer execute:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating 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 step of comparing 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 determining the unknown reaction of the compound pair with the difference values being coincident with the difference value of the known reaction as a virtual reaction;

a step of generating compound synthetic pathways by use of nodes representing the compounds and edges representing the known reaction and the virtual reaction respectively; and

a step of selecting a synthetic pathway from a starting compound to a target compound out of the generated compound synthetic pathways.

14. The synthetic pathway generating program according to claim 13, for making the computer execute a step of determining thermodynamic feasibility about the selected synthetic pathway.

15. The synthetic pathway generating program according to claim 13 or 14, for making the computer execute a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

16. A synthetic pathway generating program for making a computer execute:

a step of converting chemical structures of compounds into numerical values;

a step of creating a compound pair and calculating a first difference value by subtracting the numerical value of one compound of the compound pair from the numerical value of the other compound thereof;

a step of calculating a second difference value by subtracting the numerical value of a starting compound from the numerical value of a target compound; and

a step of generating, by use of the starting compound, the target compound and the plurality of first difference values, a synthetic pathway wherein a total value of the first difference values in the synthetic pathway from the starting compound to the target compound is coincident with the second difference value.

17. The synthetic pathway generating program according to claim 16, for making the computer execute a step of calculating a (molar) theoretical yield of the target compound synthesized by the selected synthetic pathway and

determining whether or not the calculated (molar) theoretical yield is equal to or larger than a threshold value.

18. The synthetic pathway generating program according to claim 17, for making the computer execute a step of determining thermodynamic feasibility about the selected synthetic pathway.