CLAIMS

1. ~~(Amended)~~ An interaction prediction device comprising:

a storage unit and a control unit, wherein

the storage unit includes:

a compound structure data storage unit that stores compound structure data on a structure of a compound; and

a protein structure data storage unit that stores protein structure data on a structure of a protein, and

the control unit includes:

a compound structure data acquiring unit that acquires the compound structure data on the compound from the compound structure data storage unit or predicts and acquires the compound structure data not stored in the compound structure data storage unit using a structure prediction method;

a protein structure data acquiring unit that acquires candidate protein structure data corresponding to the protein structure data on a candidate protein serving as the protein to be a candidate for interaction with the compound from the protein structure data storage unit or predicts and acquires the candidate protein structure data not stored in the protein structure data storage unit using the structure prediction method;

a predicted protein determining unit that calculates a plurality of binding strengths between the candidate protein and the compound using a plurality of docking simulation methods based on the compound structure data acquired by the compound structure data acquiring unit and the candidate protein structure data acquired by the protein structure data acquiring unit, determines any one of the binding strengths or a combination of the binding strengths as a predicted binding strength corresponding to an eventually predicted binding strength by making a

the learning method and the meta-estimation method.

6. The interaction prediction device according to any one of claims 1 to 5, wherein

the storage unit further includes:

a genetic data storage unit that stores genetic data on a gene of an individual, and

the protein structure data acquiring unit predicts and acquires the candidate protein structure data using the structure prediction method based on the genetic data stored in the genetic data storage unit.

7. ~~(Amended)~~ An interaction prediction method executed by an interaction prediction device including:

a storage unit and a control unit, wherein

the storage unit includes:

a compound structure data storage unit that stores compound structure data on a structure of a compound; and

a protein structure data storage unit that stores protein structure data on a structure of a protein,

the method executed by the control unit comprising:

a compound structure data acquiring step of acquiring the compound structure data on the compound from the compound structure data storage unit or predicting and acquiring the compound structure data not stored in the compound structure data storage unit using a structure prediction method;

a protein structure data acquiring step of acquiring candidate protein structure data corresponding to the protein structure data on a candidate protein serving as the protein to be a candidate for interaction with the compound from the protein structure data storage unit or predicting and acquiring the candidate protein structure

8. ~~(Amended)~~ A computer program product having a non-transitory tangible computer-readable medium including programmed instructions for causing, when executed by an interaction prediction device including a storage unit including a compound structure data storage unit that stores compound structure data on a structure of a compound, and a protein structure data storage unit that stores protein structure data on a structure of a protein, and a control unit,

the control unit to perform a method comprising:

a compound structure data acquiring step of acquiring the compound structure data on the compound from the compound structure data storage unit or predicting and acquiring the compound structure data not stored in the compound structure data storage unit using a structure prediction method;

a protein structure data acquiring step of acquiring candidate protein structure data corresponding to the protein structure data on a candidate protein serving as the protein to be a candidate for interaction with the compound from the protein structure data storage unit or predicting and acquiring the candidate protein structure data not stored in the protein structure data storage unit using the structure prediction method;

a predicted protein determining step of calculating a plurality of binding strengths between the candidate protein and the compound using a plurality of docking simulation methods based on the compound structure data acquired at the compound structure data acquiring step and the candidate protein structure data acquired at the protein structure data acquiring step, determining any one of the binding strengths or a combination of the binding strengths as a predicted binding strength corresponding to