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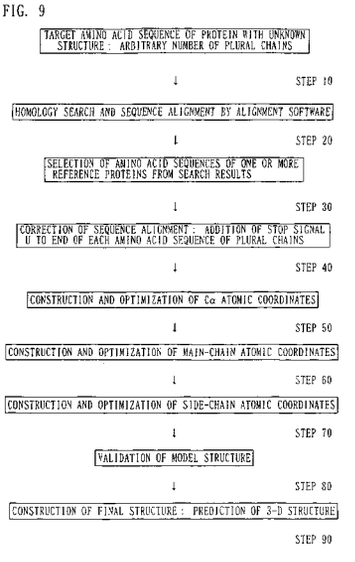
(54) METHOD OF CONSTRUCTING STEREOSTRUCTURE OF PROTEIN HAVING PLURAL NUMBER OF CHAINS

(57) A method is provided of constructing a tertiary structure of a protein composed of plural chains having given arbitrary amino acid sequences by extending an comparative modeling method of constructing a tertiary structure of a protein composed of a single chain having a given arbitrary amino acid sequence (extended modeling method). In this method, an input file format of the plural chains in a computer software program is each corrected so as to present a form of a temporary single chain (correction of sequence alignment) and the tertiary structure is constructed based on the modeling method while assuming that the structure has plural chains in calculation of a potential formula by the computer software program, thereby constructing the tertiary structure of the target protein.

Namely, a method is provided of constructing the tertiary structure of an arbitrary protein having plural chains, which serves as a particularly important key factor in developing drugs or the like, highly accurately and much more efficiently than by a conventional method.

FIG. 9



FLOW CHART SHOWING PREDICTION OF 3-D STRUCTURE OF PROTEIN ACCORDING TO THE INVENTION (EXAMPLE)

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