Many different approaches are needed to enable an expansion of the industry for drug design. Focusing on (membrane-)protein-ligand interactions it is of interest to know the structure of the target molecule. As it is known that proteins are the key-players to our functions in our organism, it is important to predict the structure of proteins. As suggested by Sanchez and Sali in their paper from 2000, there are five errors that can occur in the process of predicting protein structures by comparing models. These errors stated were “errors in side-chain packing”, “distortions and shifts in correctly aligned regions”, “errors in regions without template”, “errors due to misalignments” and “incorrect templates”. As the authors point out the significance of the side-chain and its function in protein, three papers are listed in the following literature review, that deal further with the structure of a functional (flexible) side-chain of a protein and approaches to inhibit its function. They have been extracted from Web of Science, PLOS and the main page from PubMed, using the queries “predicting protein structure”, “functional side-chain placement in proteins” and ”functional side-chains in proteins”.

In his article Canzar stated the importance of protein design in order to successfully design drugs[3]. He presented a mathematical algorithm for the exact placement of the side-chain of a protein, given only the sequence of the protein backbone.

An approach in order to design drugs is to examine the molecules that activate our target molecules[4]. Paying attention to Allison E.Kennedy’s paper, she provides a method of molecular modeling in silicio docking of the Ligands using a the software named Sybyl-X 2.1.1.

To provide precise and fast information about functionalities and structures of unknown proteins it can be helpful to compare a unknown protein-structure to already known structures. This is a main approach of Narayanan Eswar as presented in her article “Comparative protein structure modeling using MODELLER”. The main program used for her work is called MODELLER. It is used to compare the structures of two or more proteins providing information about their similarities, folding pattern of the unknown protein and possible functions.

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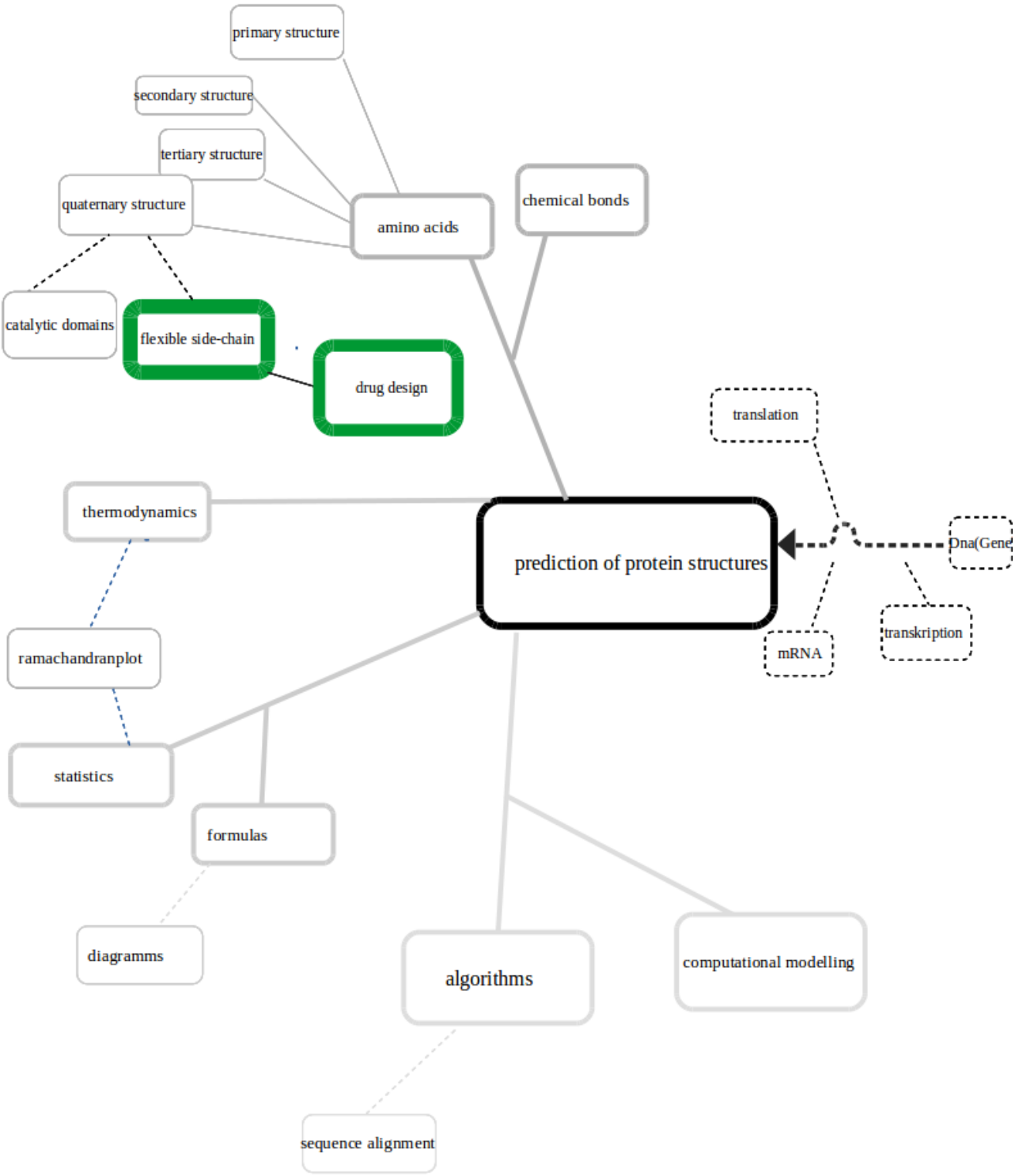
primary structure
secondary structure
tertiary structure
quaternary structure
amino acids
chemical bonds
catalytic domains
flexible side-chain
drug design
translation
thermodynamics
prediction of protein structures
Dna(Gene
transkription
mRNA
ramachandranplot
statistics
formulas
diagramms
algorithms
computational modelling
sequence alignment