Many different approaches are needed to enable an expansion of the drug industry. Setting a focus on protein ligand interactions it is important to know the target molecule, in order to create an ideal cure.

In his article „An Exact Algorithm for Side-Chain Placement in Protein Design“ from year 2011, Stefan Canzar stated the importance of protein design in order to successfully design drugs. He presented an algorithm for the exact placement of the side-chain of a protein, given only the protein backbone. Given the two assumptions, that the side-chains adopt only statistically dominant low-energy conformations and the energy of a protein is the sum of intrinsic side-chain energies and pairwise interaction energies, Canzer states that these information are not enough to predict the side-chain placement. He suggests to rather combine two algorithms named the branch-and bound algorithm and the Lagrangian relaxation approach. However this model of the side-chain placement is mathematical and should include biochemical properties to provide exact information about the side-chain placement in vivo.
Another approach in order to design drugs is to examine the moleculesthat activates our target molecule. Paying attention to Allison E.Kennedy's paper "Nerve growth factor inhibitor with novel-binding domain demonstrates nanomolar efficacy in both cell-based and cell-free assay systems", she provides a method of molecular modeling in silicio docking of the Ligands. Kennedy provides information about the interaction between the nerve growth factor(NGF), a protein that regulates the development of neurons through activation of the Tropomyosin receptor kinase A (TrkA) a trans-membrane protein. At it has been proven that elevated levels of the NGF have a negative impact on the organism it is in interest of scientist to partially hinder the affinity of NGF to the TrkA. A method suggested by Kennedy is to alter the structure of the NGF using a software named Sybyl-X 2.1.1.
To provide precise and fast information about functionalities and structures of 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 in her work is called MODELLER. It is used to compare the structures of 2 protein providing information about their similarities, folding pattern etc.
To make sure the target molecule is directly aspired and the drugs designed are as precisely targeted as possible it is important to combine these methods and approaches. Hence results of each work should be considered as equally important and should be taken into account.