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Editorial

New Pharmacology: Multi Component - Multi Protein Interaction

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Drug discovery/invention to manage/treat multifaced diseases pathogenesis is always challenging as these conditions are complex due to the involvement of multiple proteins and pathways. Further, the current choice of therapeutic agents to treat numerous diseases are single-target agents that were developed based on the concept of "*lock and key*" or "*one drug-one protein interaction*". Although these agents are effective in managing diseases and cover the major portion of the prescription they are associated with multiple severe side effects. Now in the present era, one should understand if the drugs were designed as single target molecules towards particular pharmacological activity, why these side effects occur?

Side effects can be explained as an unwanted pharmacological spectrum that gets expressed through the medication at therapeutic dose and is not intended; could be the outcome of alteration in homeostatic proteins/pathways. For example – let us assume a case in which a patient is under psychiatric illness and the physician prescribes atypical antipsychotic molecule, olanzapine. Now the olanzapine - induced weight gain is the side effect that is undesired during the pharmacotherapy of psychiatric illness. Here, one must understand, why weight gain is occurring if olanzapine was designed to target only the D_2 receptor? It means olanzapine has the tendency to interact with other protein molecules relating to weight gain or energy expenditure.

How to Deal with it?

During the pharmacotherapy of any disease, two points must be taken into prime consideration i.e. (a) medication should express the therapeutic activity and (b) it should have minimal side effects. Now if the drug is a single targeted molecule and if physician tends to minimize the side effect, he/she may reduce the dose prescribed. However, this concept may not always work since the dose may not be able to produce therapeutic effect. Similarly, if the dose is increased side effects may occur apart from the desired pharmacological activities.

This process can be explained by two events i.e. primarily, design a molecule in such a way that it specifically binds to a single protein and modulates to that extent, till the therapeutic effect is reached. However, from this process, the amount of drug/molecule required may be more and may modulate other proteins which are not desired and considered as the side effects. Secondarily, molecule(s) can be designed to target multiple proteins which are identified as "*multi component-multi protein*" interaction. In this case, the drug molecules can be designed in such a way that molecules modulate multiple proteins involved in the pathogenesis of polygenic diseases. The benefit of this approach is that a group of similar compounds can be utilized to target multiple proteins in disease pathogenesis. It means compounds are free to target multiple proteins involved in the disease pathogenesis but not homeostatic proteins.

How to Assess it?

Gene set enrichment analysis and network pharmacology can contribute to this aspect. Gene set enrichment analysis helps to predict the disease phenotype based on a large set of modulated genes by the particular compound. Any compound may or may not have an effect on a particular protein/gene which can be explained by probable activity and probable inactivity. A probable activity has been explained by few researchers as the probability to occur the positive results/expression of the protein/gene (up- or down-regulation) if the experiment is repeated for 'n' number of trials. Similarly, probable inactivity defines the measurability of negative results for the 'n' number of experimental trials. Now, if the probable activity of compound to express the particular gene is greater than probable inactivity, the gene may be expressed and the therapeutic activity may occur.

Implication in Practice

Of course, the "*multi component-multi protein*" track for pharmacological activity is slightly complicated. This is due to multiple secondary metabolites present in traditional medicinal plants and their quality control parameters do matter. However, this approach can be successively practiced in medical via the collaborative task of bioinformatics, traditional and modern medical practitioners, researchers, industrialists and sight towards "*multi-compound-multi-protein*" interaction. Today, many researchers believe this way of approach could be better than that of single-target drug

molecules and could be utilized in the pharmacotherapy of multiple complex polygenic pathogenesis.