Drug Design: Structure-Activity Relationship (SAR)

Nafiseh Bolghanabadi[1], Lili Arabuli[2]

The University of Georgia, School of Health Sciences
[1]BA student, Pharmacy Bachelor Programme in English;
[2]Supervisor, Doctor of Chemistry, Associate Professor

The structure–activity relationship is the relationship between the chemical or 3D structure of a molecule and its biological activity. The analysis of SAR enables to determine the chemical groups responsible for evoking a target biological effect in the organism. This allows modification of the effect or the potency of a bioactive compound by changing its chemical structure. Medicinal chemists use the techniques of chemical synthesis to insert new chemical groups into the biomedical compound and test the modifications for their biological effects. A Structure-Activity Relationship is the relationship of the molecular structure of a chemical with a physicochemical property, environmental fate attribute, and/or specific effect on human health or an environmental species. These correlations may be qualitative or quantitative. Qualitative predictions are based on comparison of valid measured data from one or more analogs with the chemical of interest. Quantitative predictions, on the other hand, are usually in the form of a regression equation and would thus predict dose-response data as part of a QSAR assessment.

SAR is based on knowledge of the drug's three-dimensional structure and how its shape and charge cause it to interact with its biological target. It is also important to consider that structure-based drug design aims the discovery of a drug lead, which is not a drug product but, specifically, a compound with at least micromolar affinity for a target. SAR depends on the recognition of which structural characteristics correlate with chemical and biological reactivity. Thus the ability to draw conclusions about an unknown compound depends upon both the structural features and the database of molecules. Nowadays the computer-aided drug design is used to predict the activity of a given structure. Computer programmes are able to measure comparison between probability of activity and probability of inactivity. This help medicinal chemists to direct synthesis or design for a specific disease and target.

Key words: *structure-activity relationship, drug, design, target*