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PASS APPLICATION IN R&D OF NEW PHARMACEUTICALS

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Abstract: A systematic approach through computer assisted design to identify novel pharmaceutical for research and development has been discussed in the present paper.

Introduction:

There are dozen thousands chemicals in use today and many more being synthesized. It is necessary to have the efficient methods for assessment of action of these compounds in the environment and human health. Experimental testing is both time-consuming and expensive. Thus, there is a pressing requirement for accurate *in silico* methods to predict the carcinogenicity. In this investigation, we studied how accuracy of rodent carcinogens estimation may be improved by using two different computer programs on the basis of their structural formulae.

Result and discussions

Usually, research and development of new pharmaceuticals are carried out step-by-step:

1. Disease identification.
2. Target choice.
3. Assay development.
4. Ligand design (hits).
5. Chemical synthesis and/or purchase of samples for biological testing.
6. Ligand finding (leads): in vitro testing of the required specific biological activity.
7. Ligand optimization (drug-candidates): *in vivo* confirmation of the required specific biological activity;