# Property Estimation for Chemical Product Design

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Chemical product design (CPD) involves the screening of a large number of chemical structures with the aim of identifying candidate molecules satisfying a set of desirable properties for a target product. By using this approach, it is possible to reduce the time and efforts required in product identification since lengthy and expensive trial-and-error processes can be avoided. The potential of this approach is enormous considering that there is a huge space of chemical structures in where it is possible to find new chemicals with new and/or better characteristics.

The limiting factors in the strategies for CPD are the generation of a large number of feasible chemical structures and their evaluation with respect to the desirable set of property values. In this sense, the property values need to be supplied and, since it is not always possible to find experimental values, property estimation methods are generally employed in this situation. However, most of the currently available methods do not provide reliable estimations for complex and large molecules such as those of biochemical or environmental relevance. For this reason, the application of CPD strategies has been somewhat limited since the property estimation methods employed do not allow the evaluation of a considerable number of feasible structures that may satisfy the set of desirable properties for the target product. Another important use of property estimation is the definition of the “needs” and/or qualities of the desired chemical product. These needs are normally defined through a set of properties. For example, for the design of a tape that sticks to a painted surface for a year and then can be removed without pulling off the paint, the “needs” and/or qualities of the glue are defined through a desired set of properties.

In this work, we presented a computer system in where a new multilevel property estimation methodology providing reliable and accurate estimates for complex and large molecules is integrated into a chemical product design strategy. By this way, the applicability of the chemical product design approach is expanded significantly making possible the design of a wider range of chemical structures, among which may be found new pharmaceuticals, raw materials, additives, nutritional ingredients, specialty chemicals, etc., with desirable functional characteristics, better environmental impact and efficient, cost effective production and marketing.