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(57) Abstract

According to the present invention, efficient and effective techniques for searching for chemical entities having desired properties can be provided. In a particular embodiment according to the present invention, techniques for searching a virtual library of compounds in order to identifiy component reactants which, when combined, can yield compounds having a set of desirable properties are provided. Methods and systems according to the present invention enable researchers and scientists to identify promising new chemical compounds in the search for new and better substances.

