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Exploring Ultra-Large Chemical Spaces With Genetic Algorithms

A major challenge in modern drug design is the vast number of possible molecules that have to be navigated to find a few molecules of interest for a particular project.

Robust search heuristics like genetic algorithms can elevate established methods in the realm of cheminformatics to find this figurative needle in a haystack. Our approach, Galileo, finds promising hit compounds in ultra-large chemical fragment spaces that contain several trillion molecules. These hits both have the desired properties for a drug development project and are most likely synthetically available.

We showcase an application of Galileo in a search for molecules that fulfill a given pharmacophore, i.e., the collection of properties that a molecule needs to possess for a desired biological activity.

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Keywords

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