Hurakan

Mind the Byte SCIENTIFIC CLOUD SOLUTIONS

What is Hurakan?

Hurakan is a 3D ligand-based virtual screening solution deployed over cloud technology. It is offered as SaaS (Software as a Service) paying only for the real usage of the system.

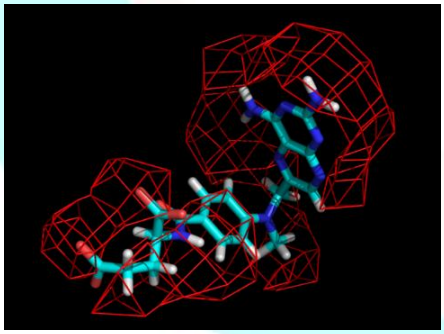
What do I need and what do I get?

You just need to provide a molecule (as a SDF file or as a SMILES string) and set a group of 1D descriptors filters in order to improve the quality of the results. Hurakan will provide you a list of potential targets with the computed activities. Once it finishes you will also be able to modify the similarity thresholds used so the activities are more influenced by certain properties of the molecule.

How does it work?

Hurakan compares molecules computing their similarity by using methods that take into account both properties of the molecule and the potential environment in which it would be surrounded when acting over a target.

With the superimposed pair, CoMSIA fields are computed at different points of a three-dimensional grid placed over the molecules. These fields take into account its position, and depending on the probe employed different physicochemical properties.



The fields are then compared, and a similarity score is computed between reference and query molecules. The screened molecules are then ranked according to the scores and those above a certain threshold are selected as hits and used to compute the potential activities of the query, weighting them by their similarity.

At the end, the user can retrieve a list of activities and modify the similarity threshold used for considering molecules as hits, and then stress the importance of certain physicochemical properties in the retrieved list of activities.

Quality of results

Using a molecule from the database as a query, after removing it from the database for the analysis, Hurakan is able to retrieve most of its annotated activities, plus potential new ones by the described method.

Compound	Retrieved	Annotated	Recovery rate
Methotrexate	159	189	0.84
Caffeine	132	145	0.91
Methotrexate *	149	170	0.87
Caffeine *	123	133	0.92

*targets with more than 100 compounds associated

Potential advantages

- It compares the behavior of the molecules with the environment obtaining non-structural biomimetic compounds
- It is a 3D method, therefore more information is taken into account, retrieving potential activities that would not appear with the classical 2D ones.
- It is a cloud tool and delivered as SaaS, you don't have to invest in software and hardware and your system will be always ready and updated growing with you.

Potential applications

- Library enrichment
- Drug reprofiling
- IP and ADME/TOX issues solving
- Elucidation of mechanisms of action.

About Mind the Byte

Mind the Byte is a research company specialized in developing and providing scientific cloud solutions for drug discovery.

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