

What is Cabrakan?

Cabrakan is a 2D ligand-based virtual screening and profiling 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?

Cabrakan can run with only a SMILE string from your query molecule and a cut-off similarity value to use as threshold for considering other molecules as hits. In the end, Cabrakan provides you a list of potential targets for the molecule (including protein targets, cell-lines and organisms) with the computed activity.

How does it work?

Being a 2D method as it is, Cabrakan computes similarity based on the Tanimoto coefficient between the fingerprints of the two molecules being compared.

These molecular fingerprints are computed with a Daylight-like algorithm, which consists in identifying and hashing topological paths in the molecule along its bonds and using them to set bits in a fingerprint, which is then condensed to a certain length and used for computing the Tanimoto similarity coefficient between molecules.

This process is repeated for both the query molecule and the nearly 1.400.000 compounds with annotated activities from the screened database, and once the similarity values are computed those above the user-defined threshold are considered as hits.

Regarding the annotated activities of the hits, activities for the query molecule are then computed and sorted by the number hits that have that activity for that target

Current Cabrakan implementation is using ChEMBLdb as an annotated database but can be used to screen other databases.

About Mind the Byte

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

Quality of results

As a case study, using a well-known antineoplastic drug such as methotrexate, which binds and inhibits the dihydrofolate reductase, we were able to re-assign said activity (P00375, P00381) based on the similar hits, as well as retrieve others such as activity against L1210 (a murine leukemia cell-line) or survival days when administrated to mice. All of the results were sustained by a high number of hits.

Target	Activity type	Value	Hits
P00375	IC50	4247.6178686 nM	59
L1210	T/C	15.6935360295 %	49
Mice	Survival days	13.2218402684	42
P00381	ID50	326.748321991 nM	39

Potential advantages

- The retrieved activities are not only related to protein targets but also include cell lines and organisms.
- Cabrakan is really fast, being able to compare a query molecule against more than 1.400.000 molecules in the database in less than 10 minutes.
- 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
- ADME/TOX issues solving
- Elucidation of mechanisms of action

Mind the Byte, S.L.
Parc Científic de Barcelona
Baldri Reixah, 4-8
08028 Barcelona

info@mindthebyte.com
www.mindthebyte.com

