

## 3D Ligand-based virtual screening solution.

*HERCULES is a computational tool which identifies non-structural analogs of a reference compound with similar biological activity and a completely different chemical structure.*

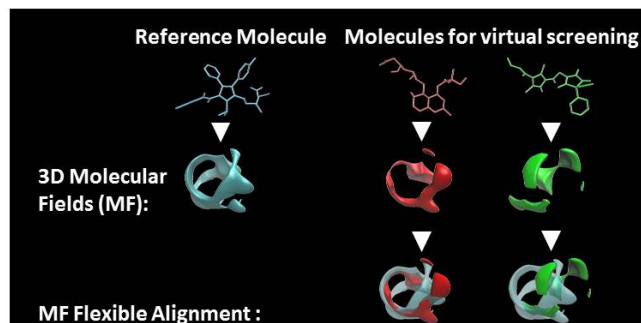
*HERCULES is offered as a service, which means that Intelligent Pharma carries out the computational part of your project in order to achieve the best outcome of your objective.*

### Working with HERCULES

We need a single active molecule which is supposed to be mimicked. HERCULES will find the best analogs within a data base which can be provided by Intelligent Pharma or by the customer.

### How does HERCULES work?

- HERCULES compares the molecular field (MF) of the reference compound with the one of any further compound in 3-D space.



- 6 MF properties are considered.
- HERCULES uses flexible MF alignment in order to scan all possible conformations to obtain the best match with the MF of the reference compound.
- HERCULES yields a list of ranked compounds according to the similarity score of the MF and gives information about the structural similarity between two compounds.

### Competitive Advantages

- HERCULES compares 6 MF properties in 3D space and considers ligand flexibility.
- HERCULES is run by Intelligent Pharma's experts so you don't need to be trained and we provide the supercomputational resources.
- Our experts identify the bioactive conformation of your molecule and can train HERCULES in respect to the project circumstances.

Developing solutions. Discovering drugs.

### HERCULES' Applications

- Drug Reprofilng.
- Hit identification.
- Determination of mechanisms of action.
- Determination of non-structural mimetic compounds.
- Solving ADME/Tox issues
- Selection of back-ups.
- Extending patent protection.
- Structure hopping.
- Construction of a pharmacophore model.
- Determination of the Bio-active conformation.

### INTELLIGENT PHARMA

Intelligent Pharma offers different services in computation aided drug discovery. Our molecular modelling department carries out research projects to help your team in designing and developing new drugs using computational chemistry & biology expertise.

**HERCULES is the most effective ligand-based virtual screening solution on the market.**

### Other technologies

#### CHIRON

Computer-aided hit to lead optimization.

#### MEDEA

A data mining solution for medicinal chemistry.

#### SELENE

Receptor-based virtual screening solution.

#### PEGASUS

2D Ligand-based virtual screening solution.

#### HYPERION

Allosteric site detector.