



Computer-aided hit to lead optimization.

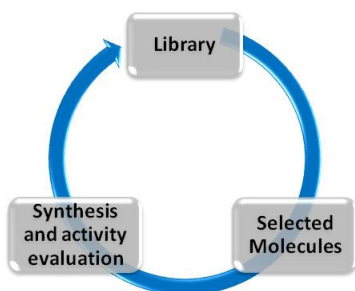
CHIRON is a technology for accelerating molecule optimization by determining the most active compounds while reducing experimental & synthesis efforts.

CHIRON 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 CHIRON

We need a scaffold for optimization.

How does CHIRON work?



- CHIRON chooses a small number of diverse molecules from the library.
- The client synthesizes and evaluates the selected molecules.
- The activity of each molecule is used by CHIRON to select the next generation of molecules.

- The client synthesizes and evaluates only the new molecules of the new generation.
- This process iterates until convergence is achieved.

Competitive Advantages

- CHIRON allows one to determine the best LEAD by only analyzing 20 % of the molecular library.
- CHIRON can optimize any molecular property by using whatever experimental data related to the chemical structure.
- CHIRON can optimize different molecular properties simultaneously.
- CHIRON identifies the majority of the most active compounds present in the molecular library.
- CHIRON determines structurally diverse molecules with high activity from the molecular library.
- CHIRON is run by Intelligent Pharma's experts so you do not need to be trained and we provide the supercomputational resources.



Developing solutions. Discovering drugs.

CHIRON's Applications

- To improve the activity of a hit.
- Hit to Lead to improve any type of measurable chemical property related to the chemical structure.
- To SOLVE:
 - ADME/Tox problems.
 - physicochemical problems.
 - low or unspecific inhibition.
- To discover new materials.

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.

CHIRON is a computational tool which can reduce up to 80% of the costs as well as time of the Hit to Lead.

Other technologies

 **HERCULES**
3D Ligand-based virtual screening solution.

 **PEGASUS**
2D Ligand-based virtual screening solution.

 **MEDEA**
A data mining solution for medicinal chemistry.

 **SELENE**
Receptor-based virtual screening solution.

 **HYPERION**
Allosteric site detector.

www.intelligentpharma.com

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