



Computed-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 works? **



- CHIRON chooses a small number of diverse molecules frim 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.

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 structure
- To discover new materials.

Competitive Advanges



- 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 simultaneosly.
- CHIRON identifies the majority of the most valuable active compounds present in the molecular library.
- CHIRON determinesstructurally 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.

Visit us!



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