scientific consulting and contract research services

cresset

Helping biotech & pharmaceutical companies succeed with chemistry

Moving from a series of screening hits to a lead compound, generating active, structurally diverse backup scaffolds or optimising those leads for the right mix of activity, ADME and toxicity properties can be highly challenging and very costly, especially if you don't succeed first time.

Companies and research groups focused on developing innovative and novel therapies often do not have the full range of expertise, software and systems required to perform compound design and optimisation in their labs. These can be highly complex tools, and knowing which solutions to choose, learning the science behind them and how to run them properly is a full time commitment that takes a level of experience and time that many labs simply cannot afford. Fortunately there is a simpler and cost effective way to access those skills.

Cresset has a long and successful track record of performing drug discovery services for our clients and collaborators. Our Scientific Consulting and Contract Research services provide a secure, confidential and cost-effective way to gain the benefit of a hugely experienced and well equipped computational chemistry team without having to run it yourself.

Moving Forward with Cresset

- Generate innovative chemical starting points for your targets.
- Optimise your lead series' activity, ADME and toxicity.
- Identify the binding mode of a target with/without a structure.
- Understand the SAR of your compounds.
- Hop between bioisosteric chemical scaffolds.

What Works for You?

All of our software and services can be accessed through a range of flexible options to suit every customer:

Let Us Do It

Our team of highly experienced computational and medicinal chemists can undertake projects of all sizes from single lead optimization studies to huge programs (our record is 40 targets in a single engagement).

Rent It in the Cloud

We have built implementations of our solutions on our private, secure Cloud computing platform. We can provide you with access to those systems and as much or little support as you require to run your jobs quickly and efficiently.

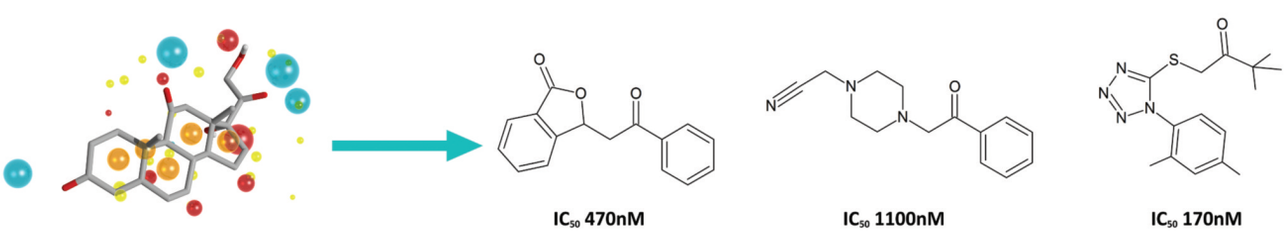
Rent It at Your Lab

We have 'Cluster on Wheels' (COW) solutions for all of our products. We build a fully working system on a portable cluster which we ship to your site. You add your data on your hard disks and run the jobs on the COW. Once complete all of your data and the results remain on your hard disks, which never have to leave your firewall.

Call Us Today to Discuss Your Projects

Example results showing structurally diverse active chemistry derived from a natural ligand.

Cortisone (natural ligand)



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Where Can We Help?

Cresset can contribute to your projects at various stages and to the degree that suits your needs. We can run whole lead discovery and optimisation projects or just help you overcome obstacles in your path. We offer solutions in a range of areas:

NOVEL TARGET

Virtual Screenlng
- Generate ideas for chemical starting points
- Identify bioisosteres in corporate or commercial compound collections
- Assess similarities of in-licensing candidates

Properties
- Generate a range of physicochemical properties for all lead compounds
- Compare alignments of new model structures or external compounds
- Suggest regions to be replaced

Scaffold Hopping
- Escape from a lead series with inappropriate SAR, ADME or toxicity
- Suggest chemically diverse and innovative bioisosteric structures

LIBRARY DESIGN → **SCREENING** → **STRUCTURE DESIGN** → **PROPERTY EVALUATION** → **LEAD OPTIMISATION** → **SCAFFOLD HOPPING**

Library Design
- Design target focused libraries
- Increase screening diversity
- Sample target specific conformations

Design
- Understand the SAR of your leads
- Generate highly innovative designs for bioisosteric molecules
- Identify the binding mode of your leads with or without a target structure

Optimisation
- Suggest changes to regions of lead structures
- Fine-tune regions of the molecules by replacing fragments
- Evaluate role of specific moieties to on- and off-target effects

NOVEL DRUG CANDIDATES

Cresset's Track Record of Drug Discovery

Cresset has successfully concluded over 100 contract research and scientific consulting projects with our customers, many of whom have come back time and time again for additional services. Because Cresset's technology can work with or without a structure of the target protein it can be used on the widest range of target classes. Example projects include:

Drug reprofiling
Focused library design
Diverse screening library design
Small molecule peptidomimetic design
Scaffold hopping
Field based pharmacophores
SAR analysis

Protein-protein interactions
Lead optimisation
Lead discovery
Virtual screening
Structure based drug design
Bioisostere detection
GPCR class A & B peptide receptors
Chemokines

Opioid receptors
Steroid receptors
Ion channels
Proteases
Matrix Metalloproteases
Protein Kinases
Sensing proteins
β-amyloid Aggregation
Antibodies
Retinoic acid receptors

Ubiquitin pathways
Patent analysis
Fragment based virtual screening
P450s
Anti-infectives
Toxicity prediction
Automated fragment growing
Fragment selection for screening

Novel anti-inflammatory target
Nuclear receptors
Design of fragment libraries
In-licensing candidate assessment
Open innovation
Nematode control agents