- Identify more effective compounds
- Speed-up compound selection
- Make decisions with confidence
- Get the most from your research

StarDrop™ 5

Software that guides you
to successful drug discovery

Introducing
the NEW module
Nova™
A new generation of
possibilities

StarDrop is a suite of software
for guiding decisions in drug discovery, helping project teams
identify high-quality compounds, fast.

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Complex, often conflicting, requirements combined with uncertain data, make it difficult to decide with confidence which lines of enquiry to pursue and which compounds to prioritise. Add to the mix, poorly balanced chemistries and lengthy, wasteful testing, and it's no surprise that most research in drug discovery results in expensive failure.

But there is an answer to these problems...

StarDrop™

StarDrop is a suite of software that helps you to deliver optimally balanced, effective drugs - fast.

By quickly highlighting diverse, high-quality compounds, StarDrop dramatically reduces the time it takes to find effective leads and then transform them into candidate drugs which will have a high probability of success downstream.

StarDrop works by evaluating complex data, which is often uncertain because of experimental variability or predictive error. In scoring this data, it brings confidence and intuitive simplicity to decision-making: guiding and validating the direction you take and which compounds you prioritise. Its instantly interactive tools then enable you to efficiently explore ways to further improve your chosen chemistries.

Highly visual and easy-to-use, StarDrop also works with your existing IT systems to integrate a multiplicity of data sources. Fully updated in version 5, it now comes with enhanced features and a unique, new plug-in module, Nova, that generates new compound ideas. Other modules include predictive ADME models, P450 metabolism prediction and automatic model building.

StarDrop – giving you the best chance yet of successful drug discovery.

Optibrium software solutions are designed to intuitively guide decision-making through complex and uncertain data.

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Create more effective drugs

Designing and selecting compounds with an optimal balance of potency, ADME and other properties is a challenge and is where so much drug discovery research fails. By highlighting high-quality chemistries StarDrop guides your research to achieve 'multi-dimensional optimisation' and targets areas of investigation with the best potential for success.

Speed-up compound selection

StarDrop dramatically reduces the time it takes to identify high-quality leads and candidates by guiding you through the maze of possibilities. Faster findings mean you can more quickly identify where balance will not be possible, confidently eliminating lines of enquiry early-on and significantly reducing wasted time. 'Virtual design' with instant, interactive feedback significantly reduces the number of compounds you need to synthesise. On top of all this, StarDrop's visual representation of data and easy-to-use interface all help you explore, evaluate and optimise your chemistries with maximum speed and efficiency.

Make decisions with confidence

StarDrop works by helping you to make objective decisions, so you can you be confident that you're making the right choices. StarDrop helps you to manage the uncertainty inherent in drug discovery data as a result of experimental variability or predictive error. Integrating data from many sources, such as predictive models and experimental assays, it scores this information, based upon specific project goals, allowing for the variability in the underlying data. This highlights any statistically significant differences, creating a solid foundation and consistent benchmark for compound analysis and selection.

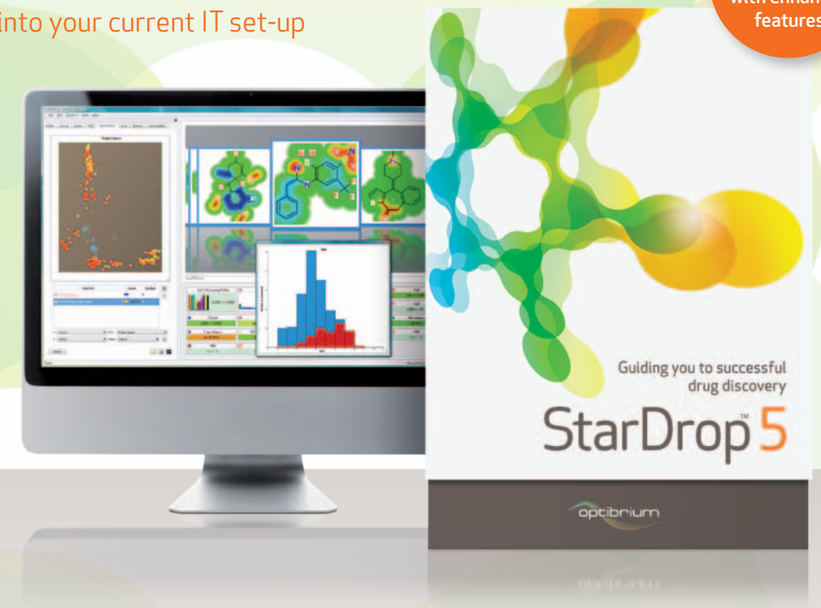
Get more from your research

StarDrop adds real value to your project by helping you to get the most from all of your resources. Seamlessly integrated into your informatics set-up, StarDrop's flexibility makes project management easier: project scientists and decision-makers can be provided with direct access to in-house models and databases. And, because the StarDrop system is modular, you only purchase the parts you need.

StarDrop 5 – bringing confidence and intuitive simplicity to your decision-making...

- Faster hit-to-lead and lead optimisation
- Design high-quality chemistries
- Dramatically reduce wasted time and effort
- Used by top 10 pharma companies and small research groups alike
- Easy-to-use, instantly interactive
- Integrates easily into your current IT set-up

Version 5:
Fully updated with enhanced features



StarDrop 5: Features

StarDrop 5 – guiding you to virtual success...

With its highly visual, easy-to-use interface, StarDrop guides you through each stage of the compound selection and design process; in guiding your decisions, its virtual environment directs you to a successful outcome

Probabilistic Scoring

Start by instantly assessing your compounds' potential for success against your project objectives

Define the profile of properties your project needs

Weight the importance of each property

Score all compounds to assess their likelihood of success

Chemical Space

Visualise chemical diversity, identify high-quality compounds, create diverse and balanced selections

Map compound scores onto your project's chemical space

Analyse the underlying property data

Select high-quality chemistries

Glowing Molecule™

Understand the relationship between properties and structure, then re-design and optimise with instant feedback

Re-design your molecules to improve their properties

Compare compounds across your data set

Visualise the impact of functional groups on a property

Highlight approaches for improving properties

For online demos, case studies and detailed information visit www.optibrium.com

A modular suite of software with a range of plug-ins...

Nova™

A new generation of possibilities

New ideas, broader horizons
Nova helps you generate new compound ideas, expand your searches, develop new chemistry strategies and find ways around patents by opening a world of opportunities in the hunt for those elusive, high-quality compounds you may have overlooked or simply not thought of.

Variations on a theme
Nova exponentially broadens your search by taking a 'parent' molecule and creating new generations of related compounds. Using a built-in collection of typical 'medicinal chemistry' transformations, Nova explores generations of potential 'children'. Nova provides an initial library of over 200 transformations for you to apply. Furthermore, using Nova you can apply multiple generations of transformations and bias selection in favour of a property or score.

New and useful compounds
Generating more choice isn't good in itself - especially if the additional choice isn't realistic. Nova creates compounds that 'make sense' from a medicinal chemistry perspective: because its transformation rules are derived from medicinal chemistry experience. Nova generates not only functional group replacements but can also make framework modifications. You can then quickly determine which ideas to focus on using StarDrop's probabilistic scoring, chemical space, Glowing Molecule and other data visualisation.

A step-change in your thinking
Nova works like a team of experts. With Nova you can apply the cumulative knowledge and expertise of many medicinal chemists to complement your thinking. By offering a completely different dimension to your research, Nova acts as a vastly experienced and creative addition to your team. Storing and applying many more transformations than a single chemist, it boosts your potential to find an optimal compound.

A flexible management tool
Nova takes full advantage of your expertise by allowing you to add and apply your own transformations, transferring your knowledge to other members of the team. It is also acts as a useful repository for knowledge, as transformation sets can be shared and 'favourites' flagged.

NEW
Contains a library of over 200 molecular transformations

Nova helps you to:
- rigorously explore the chemistry around hits
- discover lead-hopping opportunities
- generate new strategies to overcome liabilities
- identify patent-busting possibilities

P450

Quantum mechanical simulation of drug metabolism

Using StarDrop's P450 metabolism models you can quickly identify the regions of your molecules that are most vulnerable to metabolism by the major drug metabolising isoforms of cytochrome P450. StarDrop's P450 metabolism models predict the regioselectivity of metabolism. However, while valuable, predicting the relative proportion of metabolite formation at different sites on a molecule is only a partial solution to designing more stable molecules. Therefore, StarDrop's quantum mechanical approach goes beyond other methods that predict only the sites of metabolism, to provide valuable additional information on the vulnerability of each site to metabolism by CYP3A4 on an absolute scale.

Auto-Modeller™

Analyse data and produce predictive models

This module gives novice and expert users alike access to the tools needed to produce validated, predictive models. Output from the Auto-Modeller includes Glowing Molecule results.

Even if you are not an expert in modelling you can:
- Automatically generate predictive models
- Use multiple advanced modelling techniques, including Gaussian Processes, Radial Basis Functions, PLS and Decision Trees
- Train, test and validate: automatically split your data into sub-sets to rigorously choose and validate the best model
- Use a suite of built-in descriptors; MWt, logP, polar surface area and many other 2D structural descriptors are included with the Auto-Modeller

As an expert user you can also manually tune modelling methods, data sets and descriptors.

ADME QSAR

Predict key properties prior to synthesis

This module enables you to predict a broad range of ADME and physicochemical properties using a suite of high-quality QSAR models including;
- logP (Octanol/Water)
- $logD_{7.4}$ (Octanol/Buffer at pH 7.4)
- Solubility
  - Aqueous Solubility
  - Solubility in PBS at pH 7.4
- Human Intestinal Absorption
- CNS (blood-brain barrier) Penetration
- Cytochrome P450 Affinities
  - CYP2C9
  - CYP2D6
- P-gp Transport
- hERG pIC50

All ADME QSAR models provide Glowing Molecule results.

FieldAlign™

Understand and apply 3D SAR

StarDrop 5

Using technology from

cresset

StarDrop's FieldAlign module, using Cresset's molecular Field technology, provides a unique, 3-dimensional (3D) insight into the biological activity, properties and interactions of your compounds, helping to guide the design of novel, potent compounds with a high chance of success.

Understand the interactions of your compounds

FieldAlign is a powerful molecular design and 3D Structure Activity Relationship (SAR) tool that allows you to compare the molecular Fields of multiple compounds in their bioactive conformations. By highlighting both similarities and differences between molecules, FieldAlign shows you where and how lead molecules bind to their protein target. This enables you to quickly identify regions of active molecules that can be replaced to perfect the design of a new lead compound.

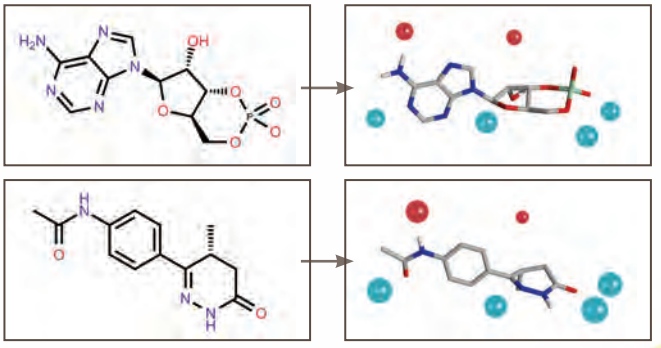
Compare compounds' Fields to find novel actives

Given the 3D structure of an active molecule and a series of 2D compound structures, FieldAlign will generate the best 3D alignment for your compounds. Every alignment is scored and ranked according to its Field similarity with the known active, so you can prioritise the compounds with the most similar activity. With this information, you can screen small compound libraries to look for novel series with greater structural diversity, or optimise the design of focused libraries for synthesis or initial screening.

Combine 3D Field similarity with other properties

You can analyse the results from FieldAlign in StarDrop's unique, visual environment and combine the Field similarities with other predicted or experimental property data. Using StarDrop's unique Probabilistic Scoring approach to multi-parameter optimisation, you can quickly target high quality chemistries with a good balance of properties for your project's requirements.

Changing the way we think and work with small molecules



Above left: 2D structures of structurally diverse bioisosteres both active at PDE3, cAMP (the natural substrate) and SKF93741, a PDE3 inhibitor

Above right: The Field patterns of the compounds reveal that they are biologically similar and share the same activity

Nova is an exciting new module for StarDrop.
A unique piece of software, Nova helps to stimulate your search for effective new compounds.
Nova sparks your imagination, exponentially opening-up your search with a comprehensive range of realistic possibilities you may not have considered.

For online demos, case studies and detailed information visit
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