Discovery Research Services

Improved decisions through predictive design

VLife's Discovery Research Services address critical situations faced by discovery scientists by providing novel and predictive solutions that facilitate better decision making at an early stage of the discovery process.

We are a research and technology development organization providing project based services for a wide range of research interests and high performance, accurate and reliable technologies for improving productivity in molecular design.

We devise and develop innovative approaches ensuring reliable solutions for complex challenges in discovery R & D. Our proven technologies create multiple design options enabling better decision making at every step in the discovery process leading to higher efficiency and productivity.

Services offerings

- Specialized Assignments
- Discovery Projects
- Strategic Research

VLife value addition

- Proven knowledge and skills
- Rapid work scope definition
- Comprehensive research
- Early stage 'go-no-go' decisions
- Improved small molecule design
- Reduction in time and cost of discovery

Customer segments

- Pharmaceuticals
- Life sciences and agri-biotechnology
- Beauty care and cosmetics
- Petrochemicals and catalysis
- Contract Research Organizations
- Research institutes

VLife Discovery Research Services

VLife's capabilities in discovery research span the early stage conceptual design and core computational molecular modeling. We offer project specific services as well as services with a long term and comprehensive discovery program perspectives.

Our knowledge of multiple domains and our cutting-edge technology platform enables us to offer services to meet complex requirements of science within affordable cost and demanding timelines. Our expertise with computational molecular design enables us to deliver results that have wide ranging applications.

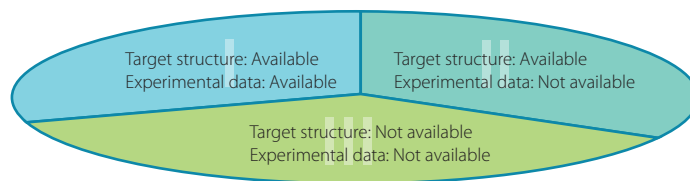| Computational technique	Results delivered	Application
Fragment based molecule design	Site specific clues for activity enhancement	Design of ligands with better activity, solving inverse QSAR problem
Property prediction	Input for QSAR or property based search	Lead profiling
Focused virtual library design	Lead candidates from most promising pools within chemical space	Improved lead candidate
Comparative binding energy analysis	Improved rationalization of activity profile	Improved understanding of docking interaction
Pharmacophore modeling	Identifying 'drug-like' parts of the molecule	Identification of novel scaffolds
Advanced database querying	Leads with similar molecular fingerprint	Scaffold hopping
Fragment based screening	Generating prioritized list of molecules with fragments of interest	Optimized input for fragment based QSAR

Complete solution for different research scenarios

Throughout the discovery cycle, researchers come across many challenging situations where informed decision making is crucial. VLife's research services address such research critical situations and help answer questions like:

- Which of the scaffolds/ molecules will get accommodated in the receptor active site?
- Where and what type of groups can we add over the scaffold?
- What is the novelty of designed scaffold/ molecule and what is scope for patenting?
- What type of groups should we add at a given position to enhance activity profile and chemical diversity?
- From activities of few molecules, can we make intelligent choices for other substitutions?
- How do we improve our lead when receptor structure is not available?
- What kind of groups should we consider for compound library generation?
- Can we prioritize novel compounds on basis of properties?
- What are the fundamental molecular properties controlling a reaction mechanism/ profile?
- Can we predict molecular properties of a new material and its likely application?
- How do you move ahead when the molecular docking energies do not correlate with the experimental activities of the ligands?
- What are the molecular properties tuning catalyst activity and what are the design aspects of novel catalysts?
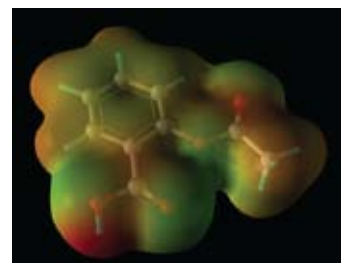
Our discovery research solutions focus on three major scenarios to ensure that all possibilities in the molecular discovery process are addressed.

Target structure: Available	Target structure: Available
Experimental data: Available	Experimental data: Not available

Target structure: Not available
Experimental data: Not available

Specialized Assignments

Tailored to meet unique challenges

As part of their discovery research programs scientists are often presented with problems that are specialized. Researchers with in-house design programs also many a times face challenges that are critical to the overall success of the program. Such challenges could be unique to that program and quite frequently could also be one-off problems. Our Specialized Assignments based services can offer solutions for situations exactly like these and are thus demand or requirement specific.

Specialized assignments are available within the following broad domains.

- Analysis of molecule – target interactions
- Specific aspects of drug repurposing
- Pre laboratory verification/ prediction/ rationalization of solutions through application of in silico techniques
- 'What-if' scenario analysis
- Catalyst improvement for improved processes
- Enzyme applications in pharmaceutical and non-pharmaceutical sectors

The above is just a representative listing and we will be happy to discuss unique and specialized problems and assess if our computational discovery expertise can help solve such problems.

Discovery Research Projects

Research services and consulting solutions for problems within the target identification to the preclinical stages of discovery research

Our Discovery Research Project services are built on methodologies that have been proven to be effective and draw upon unique techniques such as molecular design based on group based QSAR. Typically our scientists can help by providing solutions in the following areas.

- Fragment based molecule design
- Lead characterization
- Fragment based screening
- Pharmacophore guided molecule design
- Target identification

- Ligand efficiency
- Lead generation
- ADMET prediction
- Scaffold hopping
- Target validation

- Lead optimization
- Focused virtual library design
- Compounds prioritization
- Structure based search

The above are representative areas only and we will be glad to discuss how we can work within similar areas of computational molecular modeling and prediction to solve discovery research problems.

Strategic Research

Our Strategic Research Services deliver long term projects with an end-to-end perspective and a high ROI. These services are usually objective specific resulting in a usable outcome over few years. Our offerings in this segment are:

NCE research
Our NCE research services offer customers the power of computational modeling from designing a new lead molecule to a studied evaluation of its chances of success in later development stage.

ChemDiagnostics®
Assessing the risk/ benefit ratio for any novel compound during the early drug development stage

IndiSwitch®
Discovery of new indications for existing drugs by design

ReViva®
Exploring new potential therapeutic targets for 'failed' molecules

Custom specific research
For conceptual discovery research projects that are expected to culminate in a defined outcome over few years

Proprietary technologies

Our scientific team that delivers research projects is equipped with the NewEdge™ technology platform, an advanced computer aided molecular design technology for molecular level studies and analysis. Exclusive and novel methodologies within NewEdge provide unique advantages to our scientists to improve outcomes from discovery projects. These methodologies have been developed by these very scientists, who are thus best placed to optimally utilize the technology's strengths for meeting project objectives.

Our technologies have been effectively employed on a variety of discovery projects and currently include the following.

VLifeMDS® : Comprehensive solution for end-to-end computer aided drug and molecular discovery having separate modules for specific tasks including molecular modeling, simulation, analysis, visualization, interpretation and prediction.

QSARpro® : Special purpose software for extensive QSAR studies with multiple methods for variable selection and statistical regression.

BioPredicta® : Special purpose software for performing biomolecule related activities such as homology modeling, protein analysis and studies of protein - ligand interactions.

ChemXplor™ : Chemoinformatics software for managing large datasets and making multiple searches on data based on 2D or 3D structures, descriptors, fingerprints and receptor properties

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vLife
adding value to life