QUANTITATIVE MEDICINE
Transforming Drug Discovery™

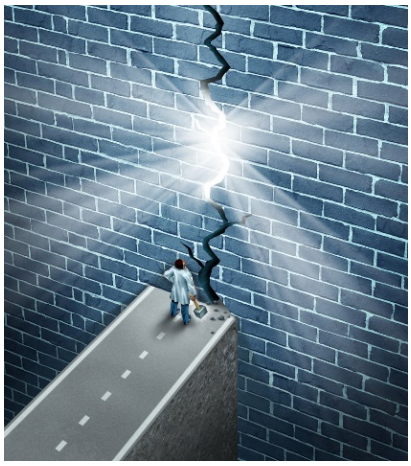
# Computational Research Engine™

## *The Lean Drug Discovery Solution*

The *Computational Research Engine™ (CoRE™)* is a dynamic drug discovery platform that iteratively optimizes prediction models using guided selection of experiments to efficiently deliver highly accurate predictions and to effectively enable better strategic decision making.

**Capabilities:**

- Experiment and compound prioritization
- Ensemble-based prediction
- *Active* Machine Learning
- Data augmentation



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Lean Drug Discovery eliminates inefficiency by increasing knowledge gains through extensive utilization of historical data and direction of new experiments to generate enriched knowledge.

This easy-to-implement solution complements existing discovery workflows and can be quickly integrated into both new and existing campaigns. *CoRE™ concurrently* optimizes the entire set of defined lead candidate properties and is proven to be effective in all the preclinical phases of small molecule drug discovery including hit finding, lead optimization, safety and *in vitro* to *in vivo* translation across all therapeutic areas.

**The *CoRE* platform**:

- ✓ **Enables** efficient discovery cycles by rapidly generating high accuracy predictions. Guided selection of experiments *minimizes* testing resources while *maximizing* knowledge gains.
- ✓ **Utilizes** substantial computational horsepower to select the most accurate predictive models from thousands generated using a comprehensive battery of machine learning algorithms and protocols resulting in superior prediction accuracy.
- ✓ **Increases** predictivity of the models by leveraging a 200M+ historical *KnowledgeBase™* of experimental results spanning many therapeutic areas from sources such as HTS, HCS, *in vivo* tests, preclinical and clinical trials to identify relevant focused datasets and augment project data.
- ✓ **Improves** the knowledge gained in each discovery cycle measurably to quickly focus resources and efforts on the most promising candidates thus ensuring a successful campaign while realizing significant reductions in time and resource costs.

Unique among *in silico* platforms, *CoRE* uses computation to effectively guide experimentation rather than substituting experiments with predictions.

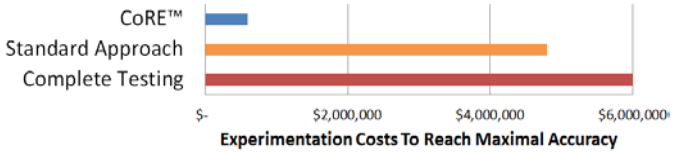
| **Proven Value to Industry and Academia** | |
|---|---|
| **Unique Features and Benefits** | **Economic Value** |
| Generate more accurate predictions with less experimentation | Reduce time, lower cost |
| Leverage historical data concurrently across assays | Avoid redundancy |
| Build more informative datasets for future campaigns | Maximize data value |
| Continually learn more accurate predictive models | Increase *in silico* model value |
| Direct experimental efforts to the most promising and relevant candidates | Minimize waste |
| Apply across campaigns or with collaborators to enable knowledge gains upstream and downstream | Reduce late stage attrition |
| **Enable Better Decisions, Cheaper and Faster** | |

## Demonstrated Success and Value Captured

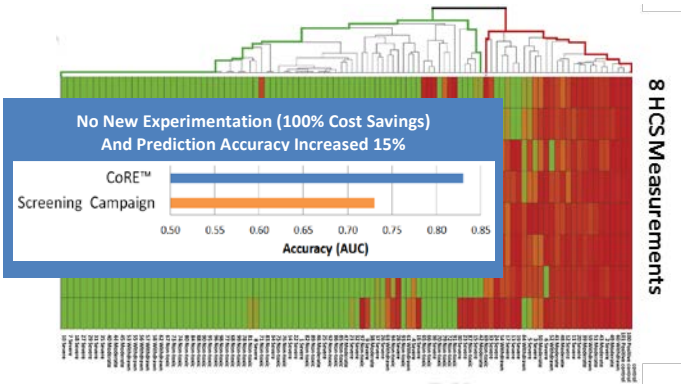
Successful collaborations with industry:

- 90% reduction in screening costs,
- 50% reduction in compound synthesis,
- 60% reduction in pre-clinical development,
- positively reduced late stage attrition risks.

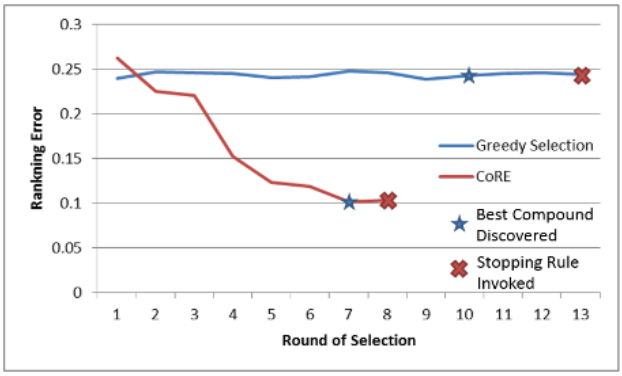
✓ For **lead series optimization campaigns** with a budget of $10 million, *CoRE* can capture $9 million in cost reductions and shave 2 years from the 5 years currently required for pre-clinical drug discovery research.




✓ For **generation of predictive *in vivo* toxicity models**, *CoRE* often requires no new experimentation to build predictive models with greater accuracy over those built using *in vitro* data including data intensive platforms such as HCS screens, saving $2-3 million in compound supply, testing and analytics.




✓ In campaigns to **optimize efficacy and eliminate multiple toxicities concurrently**, CoRE has demonstrated reductions of 40% in synthesis and 30% in screening compared to standard methods.




## *CoRE* – An Industry First

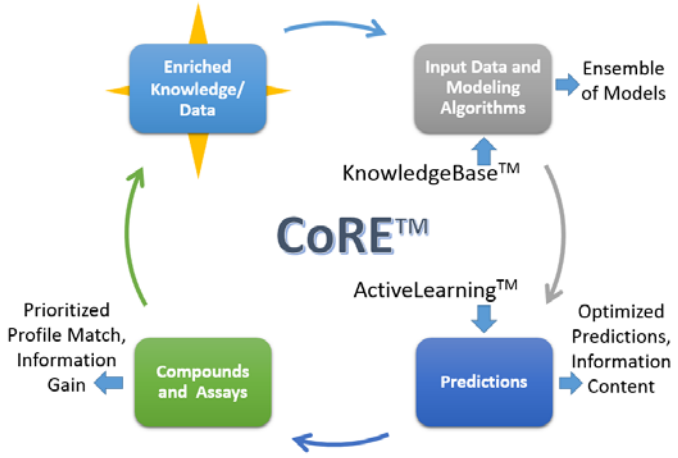
✓ ***CoRE*'s polypharmacological approach builds a comprehensive set of predictive models** from many feature sets and multiple algorithms to identify and apply the best predictive algorithms specifically matched to the problem.

✓ ***CoRE*'s *KnowledgeBase*™ utilizes over 200 million experimental results** spanning many therapeutic areas and millions of compounds to improve prediction accuracy for any assay.

✓ **Patented *ActiveLearning*™ enables large-scale hypothesis testing** for optimal experimental design while substantially reducing experimentation.

✓ **Utilizing knowledge from thousands of diverse experimental sources**, CoRE efficiently identifies compounds with optimal drug-like properties, while *minimizing off-target effects*.

✓ **Simple and fully automated workflow** allowing seamless integration into any drug discovery and development process.




**We welcome your inquiries and offer you the opportunity to learn how effectively *CoRE* can transform your discovery efforts!**

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