What if you could identify **more potent** and **diverse** hits and leads and **avoid** late stage failures?

It takes about 10 to 15 years and more than a billion dollars to bring a new drug from initial discovery to FDA approval[1] and can be as high as $11 billion.[2]

For every 5,000 to 10,000 compounds that enter the pipeline, only one receives approval.[1]

Lack of efficacy is the most frequent cause of failure in drug development.[3]

Introducing TIDEA™*

- Target-independent approach to predicting small molecule drug candidate affinity
- Effective for multiple targets, molecular shapes and scaffolds
- Can be used to select molecules with high affinity without sacrificing chemical diversity
- Addresses primary reasons for lack of efficacy: low potency or incorrect molecular mechanism of action

Benefits of TIDEA™

Identifies Diverse Leads with High Affinity

Affinity is critical for efficacy.

Greater diversity leads to more back-up scaffolds and stronger IP.

Provides more choices, allowing you to raise the ADMET cutoff during lead optimization.

Avoids Failures Due to MMOA Assumptions

Unlike structure- and ligand-based virtual screening methods, TIDEA does not rely on assumptions regarding molecular mechanism of action.

Focus Time and Resources

Identification of a more potent and diverse subset of molecules allows you to focus precious time, synthetic chemistry and screening resources on the most promising candidates.

1. Pharmaceutical Research and Manufacturers of America, 2013 Biopharmaceutical Research Industry Profile
2. “The Truly Staggering Cost of Inventing New Drugs” Forbes, February 10, 2012
3. Kola and Landis, Nature Reviews Drug Discovery **3**, 711-716 (August 2004)

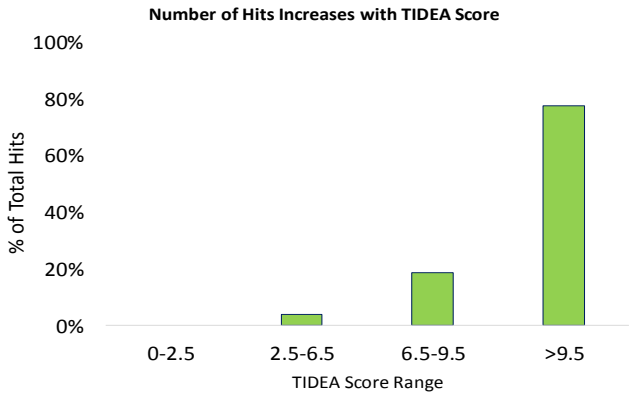
*Target-Independent Drug Enhancement Algorithm

Choose the Right Molecules in Discovery

Increase Hit Rates with TIDEA™

An independent, prospective trial at University of Michigan demonstrated that high TIDEA values predict activity and can be used to increase hit rates.[1]

The study also showed that TIDEA can reduce cost of chemical purchase, synthesis and screening by 40% while maintaining 96% of the hits.

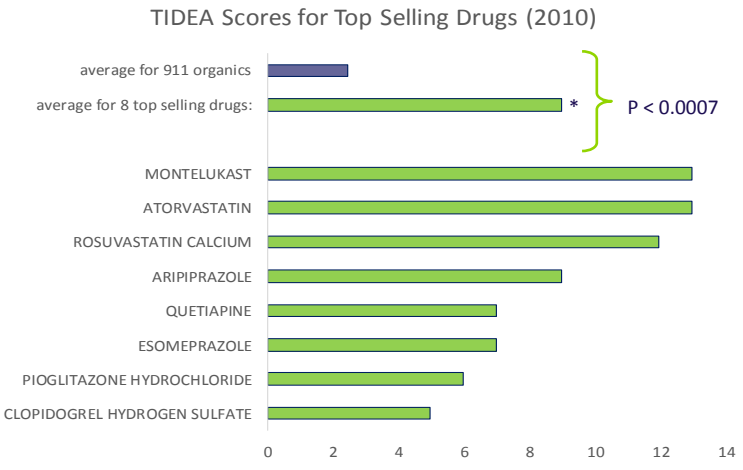


Accelerate Lead Generation and Lead Optimization

TIDEA can accelerate lead generation and lead optimization by enriching highly potent (<nanomolar) and excluding weak (>micromolar) molecules. In this retrospective study of a diverse (31 target) set of 120 bioactive small molecules, 100% of the highly potent molecules are found in the top 41% of TIDEA scores, while 70% of the weaker molecules are excluded.[2]

TIDEA Range	% of molecules	% Highly Potent (Ki≤ 1nM)	% Weak (Ki≥1000nM)
0 to 8	59%	0	**70%**
9 to 16	41%	**100%**	30%

Increase Your Chances of Success in Development



TIDEA Distinguishes Successful Drugs from Non-Drug Molecules

Average TIDEA scores are significantly higher (8.3) for 8 top-selling small molecule drugs* than for a set of 911 commercial organic molecules (2.2) selected from the Available Chemical Directory.[3,4]

* Two of the top ten drugs in 2010 were not small molecules

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FOCUS SYNTHESIS

CREATIVE PRACTICAL SOLUTIONS

1. Study performed in a collaboration with Dr. Matthew Soellner, College of Pharmacy, University of Michigan (unpublished data)
2. Structures and data from Binding Database, Chen,X., et al. Bioinformatics 18:130-139 (2002); Liu,T.,et al., Nucleic Acids Research 35:D198-D201 (2007).
3. Top 8 selling small molecule drugs in 2010: http://www.reuters.com/article/2010/04/13/roche-avastin-drugs-idUSLDE63C0BC20100413
4. 911 organic molecules were obtained from the Available Chemicals Directory: http://accelrys.com/products/databases/sourcing/available-chemicals-directory.html