KEBOTIX

Materials for tomorrow, TODAY

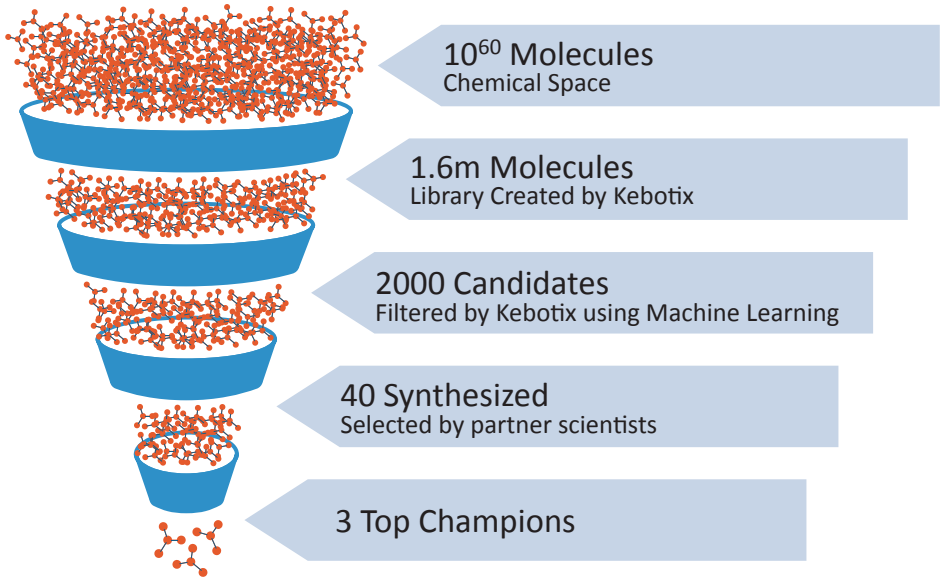
Kebotix Case Study:
High-Throughput Virtual Screening

A virtual study combining deep learning, domain knowledge and quantum chemistry identified new classes of blue OLEDs with excellent optical properties and chemical stability.

Summary Highlights

- Collaboration between Kebotix's parent lab at Harvard and Samsung.
- Identified 2,000 novel blue OLED candidates from a library of 1.6m molecules.
- Generated property prediction models using only publicly available sources.
- Incorporated domain expert knowledge by asking scientists to "vote" on viability of candidates proposed by high-throughput virtual screening (HTVS).
- Kebotix vision: Integrate powerful HTVS software with robotic hardware currently used in commercial-scale labs.

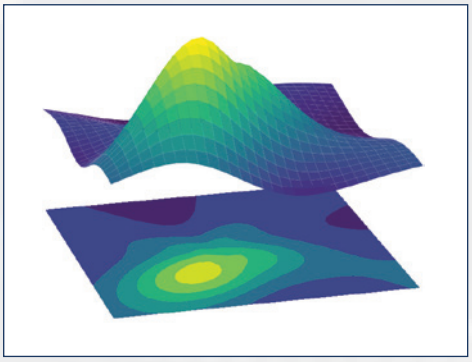
Virtual Screening Funnel



Next-Generation HTVS

Kebotix has tackled hardware and software bottlenecks to make HTVS standard for large-scale R&D

1. Paired HTVS with high-through put lab robotics to create the closed loop discovery
2. Reduced the number of quan-tum/DFT calculations required for data enrichment



3. Improved chemical libraries using generative models

Who We Are

Kebotix (www.kebotix.com) is a platform company for chemicals and materials ushering in a new age of high-speed innovation using artificial intelligence and robotic automation. Kebotix has built the world's first self-driving lab for materials discovery powered by AI and robotics. Kebotix, founded in 2017, is accelerating the exploration, discovery, use and pro-duction of new molecules and materials that can solve some of the world's most urgent problems.

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Using Breakthrough Methodology

Alán Aspuru-Guzik, Kebotix's Chief Visionary Officer, and three post-doc students from Harvard Chemistry and Chemical Biology demonstrated the feasibility of "needle in a haystack" virtual screening methods for identifying new thermally activated delayed fluorescence (TADF) OLED materials. Using quantum chemistry calculations in combination with machine-learning predictions, the team evaluated relevant TADF-properties of hundreds of thousand candidates in the screening library. The number of required computationally expensive calculations was reduced by developing a neural network for pre-screening of TADF properties. The neural network consists of two hidden layers and 100 rectified linear units (ReLUs) each, enabling identifying correlations between SMILES chemical structures and the fluorescence rate constant (kTADF). Out of 2,000 lead candidates generated during the study, domain experts voted on 40 candidates to be synthesized in a lab. The synthesis elucidated three "champion" molecules with high potential for further development. The HTVS study also identified existing and well-known TADF emitters, confirming that the screening methods were consistent with domain.

[1]Design of efficient molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach (Nature Materials, August 2016)

Who Benefits from HTVS?

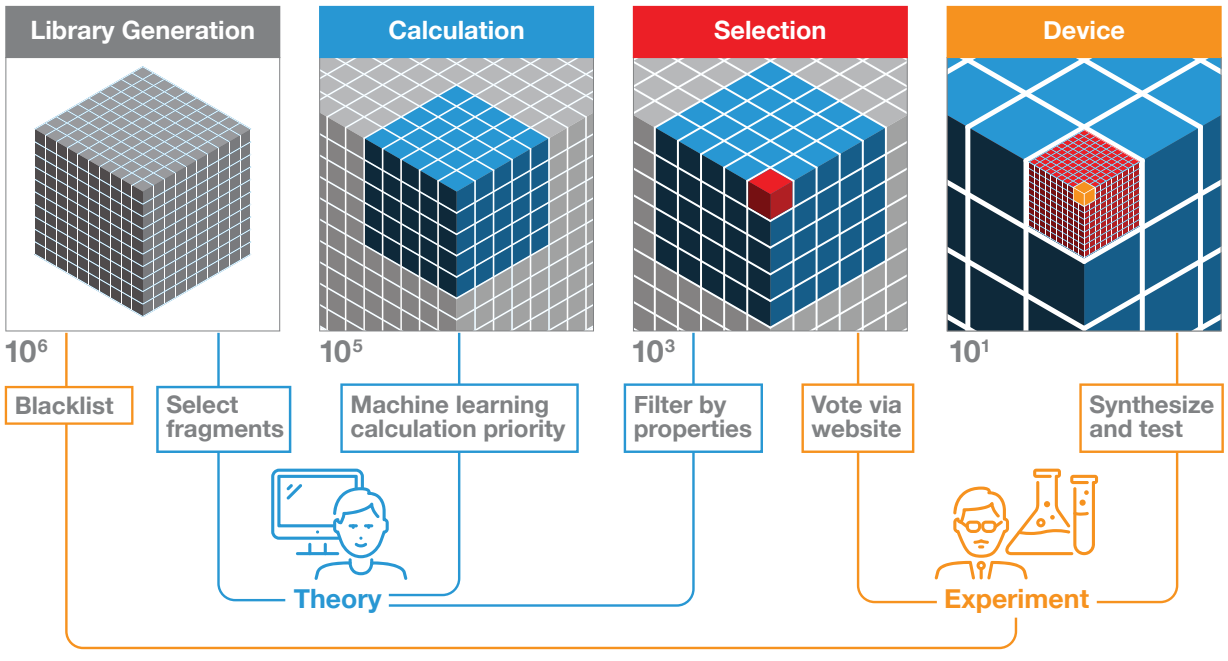
HTVS is useful for tackling tough chemistry problems across industries. Applications include:

- Increasing lubricant viscosity via functional group substitution
- Finding green solvents with lower disposal/reprocessing costs
- Identifying non-toxic pesticides with higher efficacy and lower unintended impact
- Reducing lead identification time for small-molecule drugs

Kebotix has been improving the speed and computational efficiency of HTVS through AI/ML. Our platform can already predict 100 novel high-performing molecules per week. To ensure quality results, we engage clients at every step and include domain experts in the HTVS feedback loop.

How can Kebotix help your company find the next blockbuster molecule?

Virtual Screening Process



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