

## Kebotix Case Study: Structure-Function Relationships

### Summary Highlights

- Predicted viscosity, boiling point and melting point for ~2,300 molecules in a screening library.
- Six identified candidates were experimentally verified, and four satisfied the client's target property profile.
- Kebotix's approach resulted in a 67% success rate, a 9-fold increase over the traditional approach.
- Produced a user-friendly HTML look-up table with a set of evaluated properties for the full library.
- Kebotix's vision: Use SFR prediction to accelerate combinatorial screening studies.

### The Challenge

Our partner needed to significantly reduce the required experimental testing to develop new classes of lubricants for automotive refrigeration systems.

### The Solution

Kebotix evaluated a library of ~2,300 potential lubricants built from a combination of 15 fragments. A set of probabilistic ML models was generated by Kebotix and validated with about 50 measurements that the partner provided.

To train the model, Kebotix augmented the partner's data with an in-house library of 3,000 relevant

molecules using a proprietary selection algorithm.

The partner brought in a team that used the cross-validated models to predict viscosity, boiling point and melting point for the set of ~2,300 molecules, narrowing down the library to 10 lead candidates.

Results were organized on an HTML interface that provided R&D scientists detailed property prediction data and 3D structure representations of each lead candidate. Six of the top performers were synthesized and tested by our client. Four of them satisfied the desired target property profile specified by the client. (See Exhibit 1 below.)

#### Exhibit 1:

Example structures with predicted properties and accuracy estimates:

Compound	Viscosity % Error (Predicted vs. Measured)	Within Customer Targeted Viscosity Range
1	4%	●
2	>100%*	●
3	>100%*	●
4	13%	●
5	29%	●
6	10%	●

\*There were "synthetic difficulties" when preparing compounds 2 and 3.

### The Story

By partnering on the discovery of new lubricants compatible with next-generation refrigerants based on environmentally friendly hydrofluoroolefins, Kebotix and a leading global provider of products and solutions across multiple industrial sectors, are integrally aligning a current project with United Nations Sustainability Goals around climate change and energy, and other global environmental efforts.

While details of the collaboration are being kept confidential for now, as is the name of the partner, Kebotix is sharing its excitement over not only

*"We built a database that our AI brain then learned from, saving our partner considerable time and money."*

—Christoph Kreisbeck, Kebotix CPO

engaging in corporate citizenship tied to researching new lubricants for automotive refrigeration systems, but for dramatically reducing the time required to come up with new chemicals. Central to this increase in the speed of discovery is Kebotix's artificial intelligence and virtual screening that combines probabilistic Machine Learning (ML) and engineering expertise.

Kebotix evaluated a library of several thousand potential lubricants. From there, a set of probabilistic ML models was generated and validated with measurements provided by the partner. The Kebotix team used the validated models to predict functional properties for the large set of molecules, narrowing down the library to a couple hundred of lead candidates. The next steps are proprietary, but the enthusiasm isn't.

"What we are doing together is magic – disrupting how R&D is done while reducing the cost and increasing the speed to bring products to market faster," says Christoph Kreisbeck, Kebotix chief product officer.

## Research's Beneficial By-Product

Not lost on Kebotix and the partner is the opportunity to help solve one of the world's most urgent problems by accelerating the exploration, discovery, use and production of new molecules and materials. Two of the UN Sustainability Goals, in the areas of energy and climate change, are being addressed in their materials discovery work focused on refrigerants.

"One goal is to take urgent action to combat climate change and its impact, and another is to ensure access to affordable, reliable, sustainable and modern energy," says Kebotix CEO Dr. Jill S. Becker. "Our work adheres to both goals set by the UN. This is by design per our corporate mission to change the paradigm of chemicals and materials discovery through AI and automation technology."

Refrigerant management is among the markets in which Kebotix is leading the chemicals and materials industry toward a new age of high-speed innovation. It also tops Project Drawdown's list of global solutions to mitigate climate change in terms of estimated atmospheric CO<sub>2</sub>-equivalent reductions between 2020 and 2050. Considered the most comprehensive plan ever proposed to reverse global warming, Project Drawdown gathers a qualified and diverse group of researchers from around the world to identify, research, and model the 100 most substantive, existing solutions to address climate change.

## How SFRS Can Benefit You

SFR is useful when finding that the right property profile is challenging and requires some amount of experimental testing (>40 measurements). SFR extracts hidden correlations to predict the macroscopic properties of all compounds in the screening library. SFR supports scientists in their domain knowledge-based rational design and helps them prioritize their selection of experimental testing to

get to the final product faster. SFR is beneficial across industries.

## Applications Include:

- Accelerating lead ID for drugs via functional group substitution.
- Tuning glass transition temperature (T<sub>g</sub>) of copolymers.
- Improving electrical conductivity of conjugated organics.

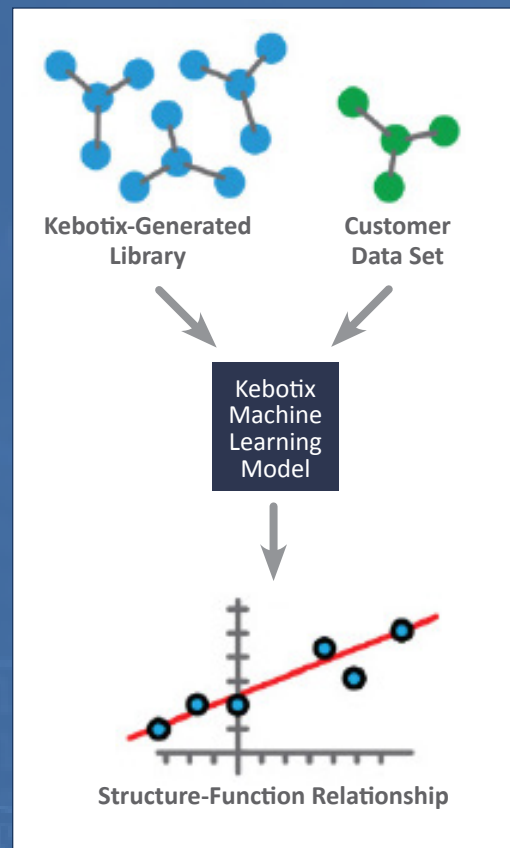
## Products to Market Acceleration



The Kebotix Platform: Rapid Discovery of Chemicals & Materials

## Presentation of Data

The Kebotix platform quickly identifies valuable SFRs that reduce cost of experimentation



## Who We Are

Kebotix ([www.kebotix.com](http://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 production of new molecules and materials that can solve some of the world's most urgent problems.