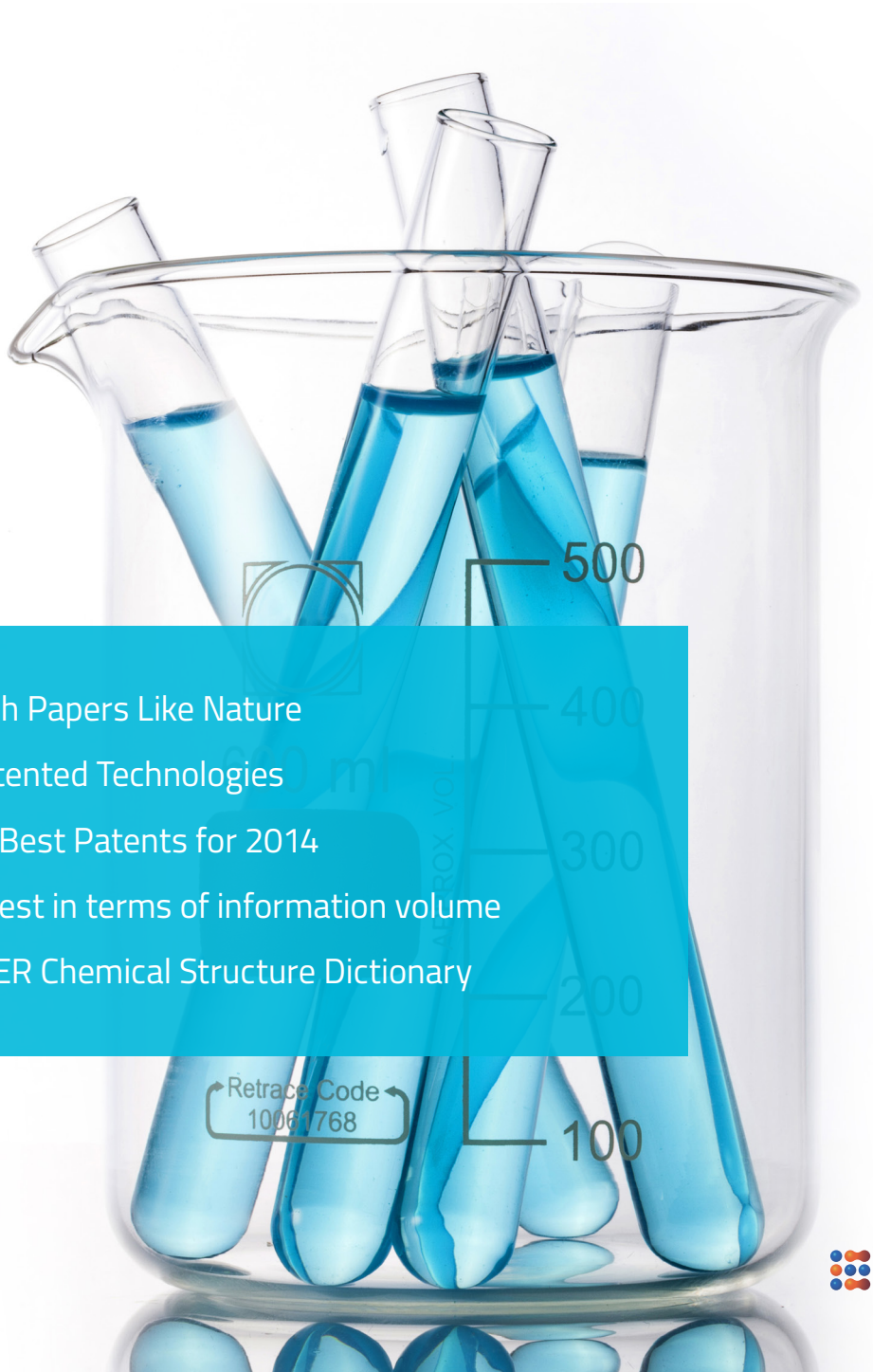
MOL Instincts

Introduction of Chemical Property Database

Mol-Instincts

First chemical database based on Quantum Chemistry.



Cited in Research Papers Like Nature

Based on 41 Patented Technologies

Awarded Korea Best Patents for 2014

The world's largest in terms of information volume

Developed NAVER Chemical Structure Dictionary

ChemEssen

What is **Mol-Instincts**?

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Based on **41 Patented Technologies**

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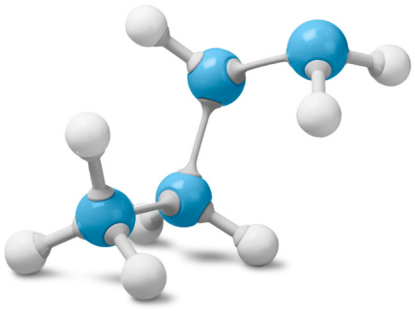
World's Largest in Terms of Information Volume

Developed **NAVER Chemical Structure Dictionary**



NEW

A New Chemical Database

World's First chemical database based on Quantum Chemistry.

4+ Million

More than 8+ Billion Data and Info

Over 2,100 sets of data are available for each and every 4+ million compounds.

95%

High Level of Accuracy

The level of prediction accuracy by Mol-Instincts has been verified to be above 95% in most cases when compared with experimental data available to date (other existing mothod, e.g., Joback Method provides 63% of the accuracy level for boiling point prediction).

Number of Chemical **Compounds Available**

Hydrocarbons		958,000+
Nonhydrocarbons	Hetero Compounds	1,510,000+
	Halogen Compounds	50,000+
	Extra-Hetero Compounds	10,000+
Drug-like Compounds		1,312,000+
Fuel Compounds	Gasoline	105,000+
	Jet-Fuel	171,000+
	Diesel	735,000+
	Biodiesel	672,000+
Chemical Processes	Soot Aromatic	248,000+
	Naphta	273,000+
	Combustion	1,349,000+
	Thermal Cracking	491,000+
	Catalytic Reforming	408,000+
	Catalytic Cracking	798,000+
	Hydro Cracking	768,000+
	Desulfurization	1,012,000+
	Isomerization	231,000+
	GTL (Gas-To-Liquid)	858,000+
	CTL (Coal-To-Liquid)	1,249,000+
	MTO(Methanol-To-Olefin) / MTG(Methanol-To-Gasoline)	689,000+

DATA CATEGORIES

Mol-Instincts
Information & **Applications**

Physicochemical Data

- Reaction engineering
- Chemical process design / simulation / optimization
- Energy efficiency improvement for combustion processes
- Chemical safety and regulation

Quantum Chemical Computation Data

- Optimized 3D molecular structure
- Energy level comparison among other molecules
- Speed up molecular optimization by starting from the Mol-Instincts 3D structure

Molecular Descriptors

- Obtaining descriptor values without running software
- QSPR / QSAR modeling

Pharmaceutical Data

- New drug discovery
- Drug possibility provision

Spectra Data

- Application study with IR / NMR / VCD

3D Visualization, Animation & Analysis

- Obtaining optimized molecular structure (2D/3D)
- Vibrational frequency analysis & animation
- Molecular orbitals (HOMO, LUMO)

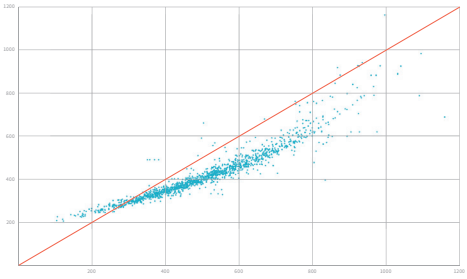
ACCURATE PREDICTION

(41 Related Patents)

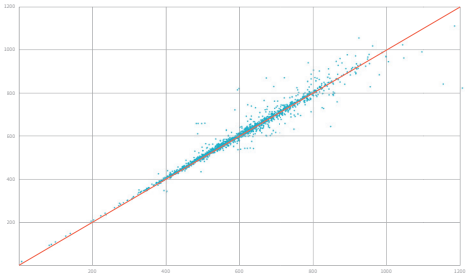
Mol-Instincts
Development Process

STEP 1	High Quality Quantum Calculation	Input structure for the quantum chemical calculation was determined by conformer analysis – the most stable structure was used.
STEP 2	Most Advanced QSPR Modeling	QSPR modeling was performed with more than 2,000 molecular descriptors which contains the quantum chemical calculation results.
STEP 3	Detailed Model Verification	Predicted data were compared and verified with the experimental data available to date, and the accuracy level of 95% was confirmed in most cases.
STEP 4	Chemical Property Categorization	The Mol-Instincts database containing over 2,100 sets of data and information per compound was constructed.

Accuracy of Existing Estimation Methods (Joback Method): **63.07%**



Accuracy of Mol-Instincts Prediction: **95.02%**



CITATION LIST

Cited in authoritative journals such as Nature.

Below is a partial list of collected citations.

PUBLISHER	PUBLICATION
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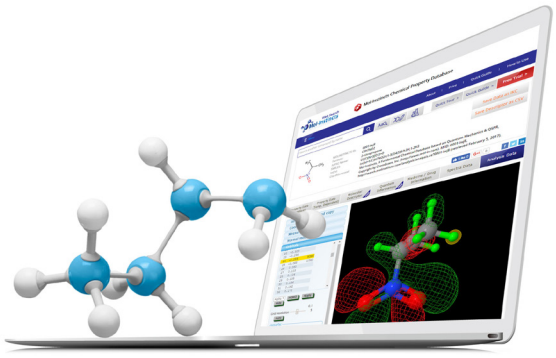
How To Use
Mol-Instincts



1	Access **Mol-Instincts Search website**.	http://search.molinstincts.com
2	**Search your compounds** by Text / Structure.	Search a Compound
3	Click '**View our data**' of the matching compound in the result list to move to the property view page.	View our data
4	**Similar compounds** are also shown along with matching accuracy.	Results with Matching Accuracy
5	**Seven different property categories** are available – simply select as needed.	View Chemical Properties

Our core technologies are
the results of fusing fundamental
chemical science and
information technologies.

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