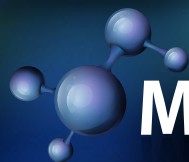




The Best Patent in 2014
S. Korea Patent Award



MOL-Instincts - Database | Predictor

Firm Foundation for Your Industrial Application and R&D Projects



ChemEssen

Mol-Instincts for Your Successful Chemical Application

What is Mol-Instincts?



A New Chemical Database

World's First chemical database based on Quantum Mechanics.



More than 2.85 Million Compounds, a Total of 10 Billion Sets of Data and Information

Over 2,100 sets of data are available for each and every 2.85 million compounds consisting of H, C, N, O, S, F, Cl, Br, I, Si, P, and As atoms.



Accuracy Level of Above 95%

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 method, e.g., Joback Method provides 63% of the accuracy level for boiling point prediction).



Free Trial for Individual and Organization

Free trial is available for anyone working in chemistry, chemical engineering, and medical researches when sign up at www.mol-in.com.

Number of Chemical Compounds Available

Free Radicals

384,000+

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) / 689,000+

MTG(Methanol-To-Gasoline)



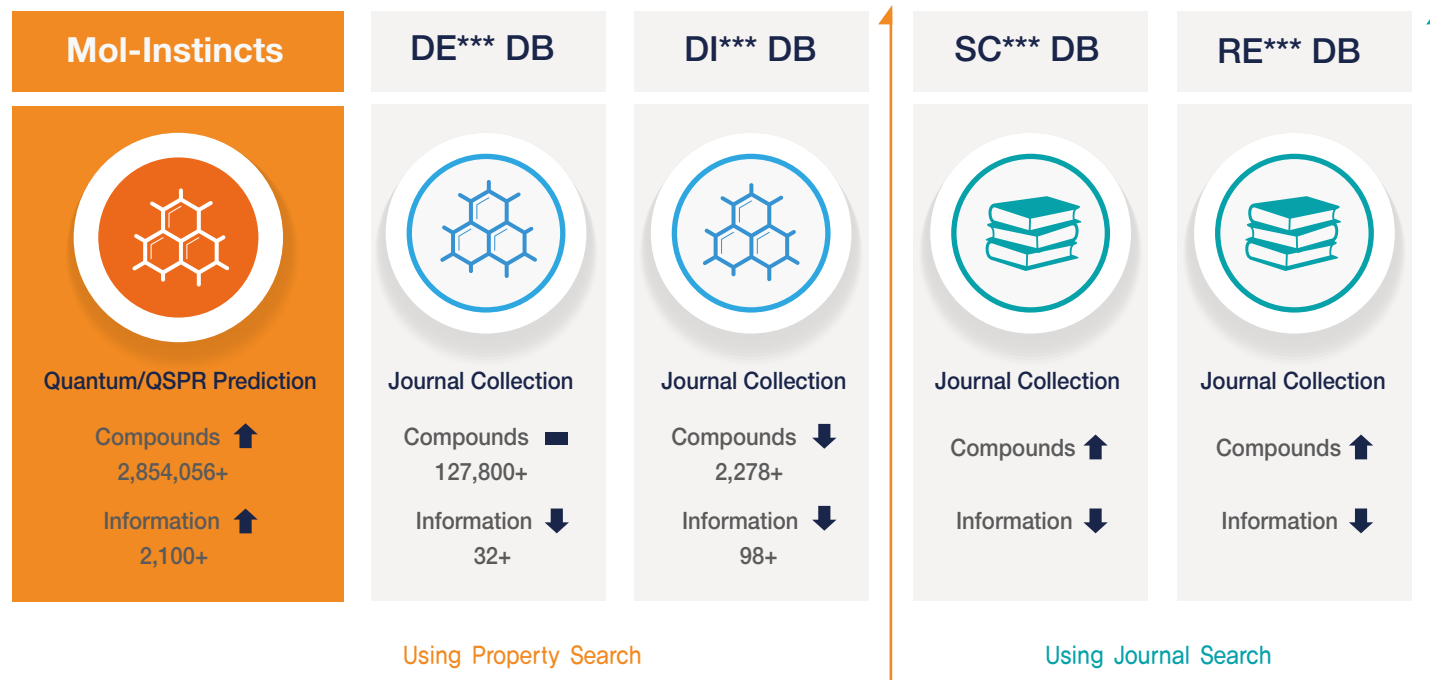
Mol-Instincts Information & Applications

Thermo-Physico-Chemical Properties		<ul style="list-style-type: none">• Reaction engineering• Chemical process design / simulation / optimization• Energy efficiency improvement for combustion processes• Chemical safety and regulation
Quantum Data		<ul style="list-style-type: none">• Optimized 3D molecular structure• Energy level comparison among other molecules• Speed up molecular optimization by starting from the Mol-Instincts 3D structure
Molecular Descriptors		<ul style="list-style-type: none">• Obtaining descriptor values without running software• QSPR / QSAR modeling
Drug-Related Properties		<ul style="list-style-type: none">• New drug discovery• Drug possibility provision
Spectra Data		<ul style="list-style-type: none">• Application study with IR / NMR / VCD
Analysis Data		<ul style="list-style-type: none">• Obtaining optimized molecular structure (2D/3D)• Vibrational frequency analysis & animation• Molecular orbitals (HOMO, LUMO)

Mol-Instincts Development Process (40 Patented Technologies)

Step ①	High Quality Quantum Calculation Input structure for the quantum 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 calculation results.
Step ③	Detailed Model Verification Predicted data were compared and verified with the experimental data available to date (collected for more than 7 years), and the accuracy level of 95% was confirmed in most cases.
Step ④	Property Categorization The Mol-Instincts database containing over 2,100 sets of data and information per compound for a variety of chemical compounds was constructed.

Mol-Instincts Comparison with Other DB Products



How to Use Mol-Instincts Database

1. Visit <http://www.mol-in.com>.
2. Sign up for **Free Trial** (a 15-day for Individual & 30-day for Organization).

3. Visit <http://search.mol-in.com>, (Mol-Instincts web search).
4. Search target compound by **text**, **2D structure**, or **properties**.

5. Click the most **matched** compound from the result list.
6. **Similar compounds** are also available along with matching accuracy.

7. **Seven different categories** are available – simply select as needed
8. More than **2,100 sets of data and information** per compound are available.

Mol-Instincts

Real Time Chemical Predictor

A New Online Predictor Available for Free



What is Mol-Instincts Real Time Predictor?



Predict Property Values for Any Chemical Compound in Real-Time

In case the desired data is not available at Mol-Instincts database, Mol-Instincts Real Time Predictor will provide the data you want via the most advanced QSPR model calculation (predictable for chemical compounds containing C, H, N, O, S, F, Cl, Br, I, Si, P or As atoms).



Free for Anyone for a Limited Time

You don't even need signup. There is no limitation or obligation.



One-Click Prediction

Simply input your chemical compound and obtain various property data instantly. It can be done with just one-click on the website, and the property data can be used for the various applications right away.

How to Use Mol-Instincts Real Time Predictor

The screenshot shows the Mol-Instincts Real Time Predictor interface. It has two main sections: 'Predict by Textual Identifier' and 'Predict by 2D structure'. The 'Predict by Textual Identifier' section has a text input field with a placeholder 'Type any identifier like Chemical Name, CAS RN, Smiles, (Standard) InChI' and a green checkmark button. Below it, there are links for 'Examples of Chemical Identifiers >' and 'Currently C, H, N, O, S, F, Cl, Br, I, Si, P and As atoms only.' The 'Predict by 2D structure' section has a 2D structure editor with a toolbar and a list of atoms (C, H, N, O, S, F, Cl, Br, I, Si, P, As) on the right. There are 'Reset' and 'Done' buttons at the bottom right.

1

1. Visit <http://realtime.mol-in.com>.

2. Define & input your compound.

The screenshot shows the 'Predicted properties of the compound entered.' section. It includes a chemical structure of benzene and a table of properties. Below the table, there are links for 'Other Names and Identifiers', a disclaimer about the prediction being based on QSPR, and a link to the Mol-Instincts Database. A table of properties is also shown.

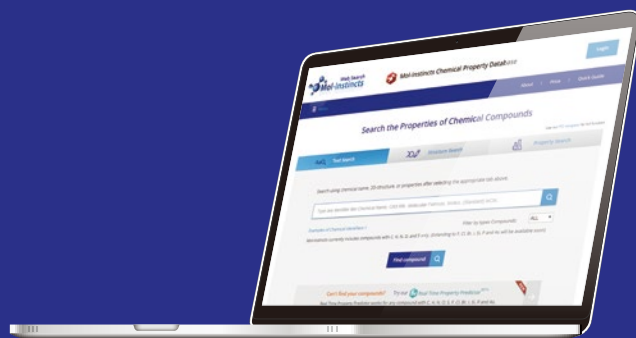
Property	Value	Unit
Absolute Entropy of Ideal Gas at 298.15K and 1bar	63.7624	cal/mol/K
Acentric Factor	0.248832	dimensionless
Critical Compressibility Factor	0.274652	dimensionless

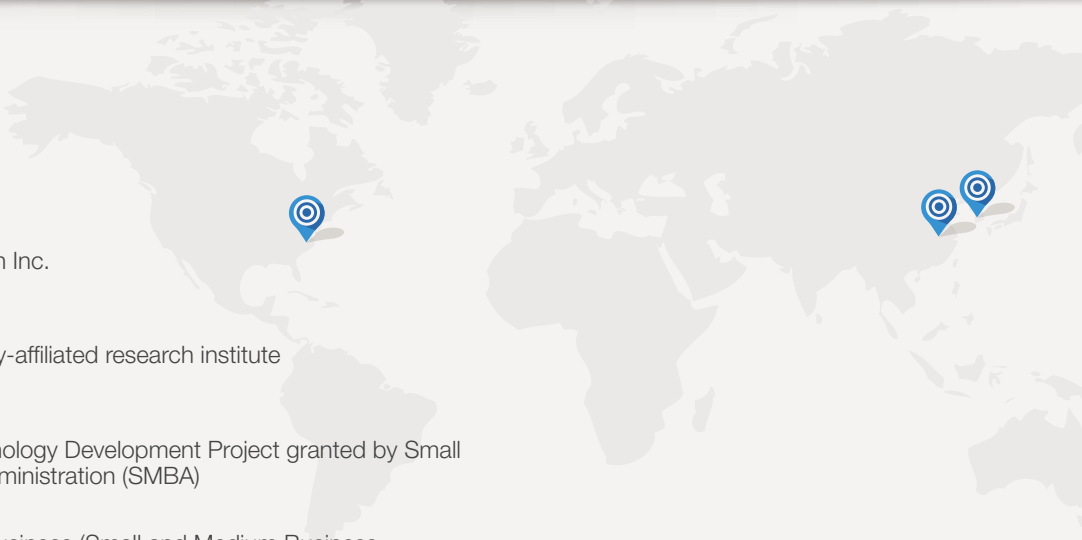
2

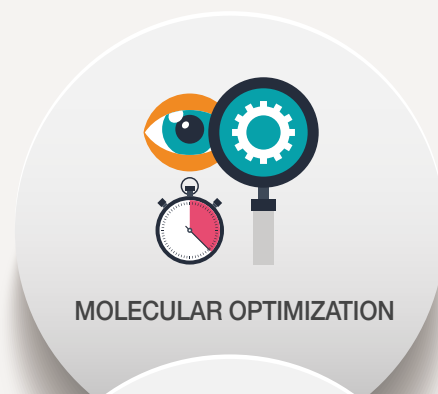
3. Obtain various physico-chemical properties.

4. A link button to the Mol-Instincts database is provided in case the input compound is available in Mol-Instincts database.

ChemEssen provided revolutionary scientific products and services for chemical industries.



- 
- 2006** Foundation of ChemEssen Inc.
 - 2007** Establishment of company-affiliated research institute
 - 2008** Awarded Innovative Technology Development Project granted by Small and Medium Business Administration (SMBA)
 - 2008** Certification for Venture Business (Small and Medium Business Administration)
 - 2009** Awarded Innovative Technology Development Project granted by SMBA
 - 2010** Launched the Beta version of Mol-Instincts Database (PC Navigator version)
 - 2011** 41 Patents granted
 - 2011** Received foreign direct investment from China
 - 2012** Registered trademark of ChemEssen for Domestic/Overseas
 - 2012** PCT International Patent granted
 - 2013** Launched Mol-Instincts Database (PC Navigator version)
 - 2014** Awarded Grand Prize for the Best Patent in 2014 by the Korea Times
 - 2014** Launched Mol-Instincts Web Search (web version)
 - 2015** Updated Mol-Instincts DB with over 2.7million compounds / Cooperation with the Korea University (CHERIC)
 - 2015** Launched Real Time Predictor
 - 2015** Processing DB update on extended atoms (F, Cl, Br, I, P, Si, and As)





Mol-Instincts **Database** -
<http://search.mol-in.com>

Mol-Instincts **Real Time Predictor** -
<http://realtime.mol-in.com>



www.ChemEssen.com

Mol-Instincts is a trademark of ChemEssen, Inc.
This product is based on a technology that is the
subject matter of a number of patent
applications.

KOREA

812, 8th Flr. AceHighTechCity 2-Cha,
25 Seonyu-ro 13-gil, Yeongdeungpo-gu,
150-096 Seoul, S.Korea

T: +82-2-3143-5933
F: +82-2-3143-5920
E: staff@chemessen.com

USA

ChemEssen, INC. Suite 1677,
1321 Upland Drive, Houston,
TX 77043 U.S.

T: +1-800-413-5613
F: +1-800-413-5613
E: staff@chemessen.com

CHINA

KOTRA 3110, Maxdo Center,
8 Xingyi-Road, Shanghai,
China

T: +86-21-5108-8771(Ext.170)
M: +86-151-2118-1868
E: china@chemessen.com