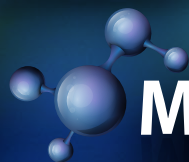




The Best Patent in 2014  
S. Korea Patent Award



# **MOL-Instincts** - Database | Predictor

*Firm Foundation for Your Industrial Application and R&D Projects*



**ChemEssen**



# 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)



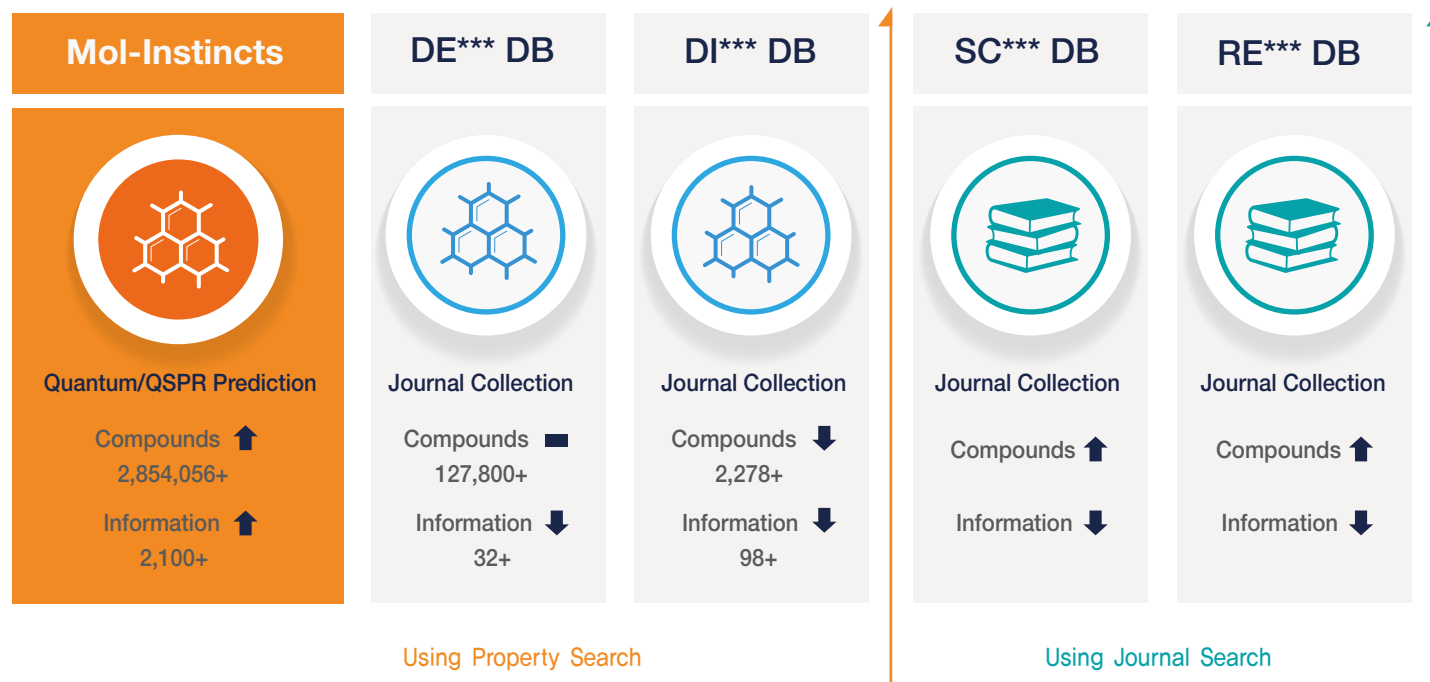
# Mol-Instincts Information & Applications

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

## Mol-Instincts Development Process (40 Patented Technologies)

Step ①	<h3>High Quality Quantum Calculation</h3> <p>Input structure for the quantum calculation was determined by conformer analysis – the most stable structure was used.</p>
Step ②	<h3>Most Advanced QSPR Modeling</h3> <p>QSPR modeling was performed with more than 2,000 molecular descriptors which contains the quantum calculation results.</p>
Step ③	<h3>Detailed Model Verification</h3> <p>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.</p>
Step ④	<h3>Property Categorization</h3> <p>The Mol-Instincts database containing over 2,100 sets of data and information per compound for a variety of chemical compounds was constructed.</p>

# Mol-Instincts Comparison with Other DB Products

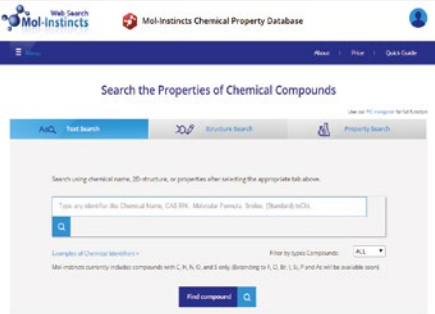


## How to Use Mol-Instincts Database



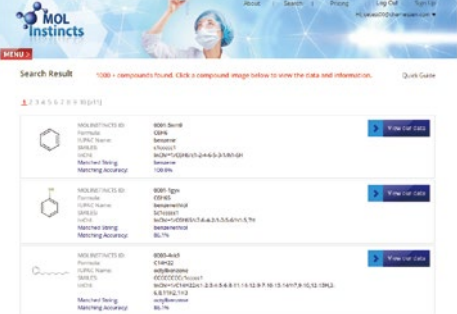
**1**

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



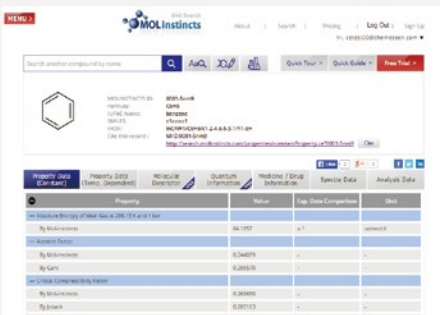
**2**

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



**3**

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



**4**

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 'Predict by Textual Identifier' section with a text input field and a dropdown arrow. Below it are '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 features a 2D structure editor with a toolbar and a vertical element palette containing C, H, N, O, S, F, Cl, Br, I, Si, P, and As. A 'Reset' button and a 'Done' button with a checkmark are also visible.

1

1. Visit <http://realtime.mol-in.com>.
2. Define & input your compound.

The screenshot displays the 'Predicted properties of the compound entered.' section. It includes a 'Predict another compound' button with a right arrow. A chemical structure of benzene is shown next to a table of properties. Below the table, there are sections for 'Other Names and Identifiers', a disclaimer about QSPR-based predictions, and a link to the 'Mol-Instincts Database' for quality-assured data.

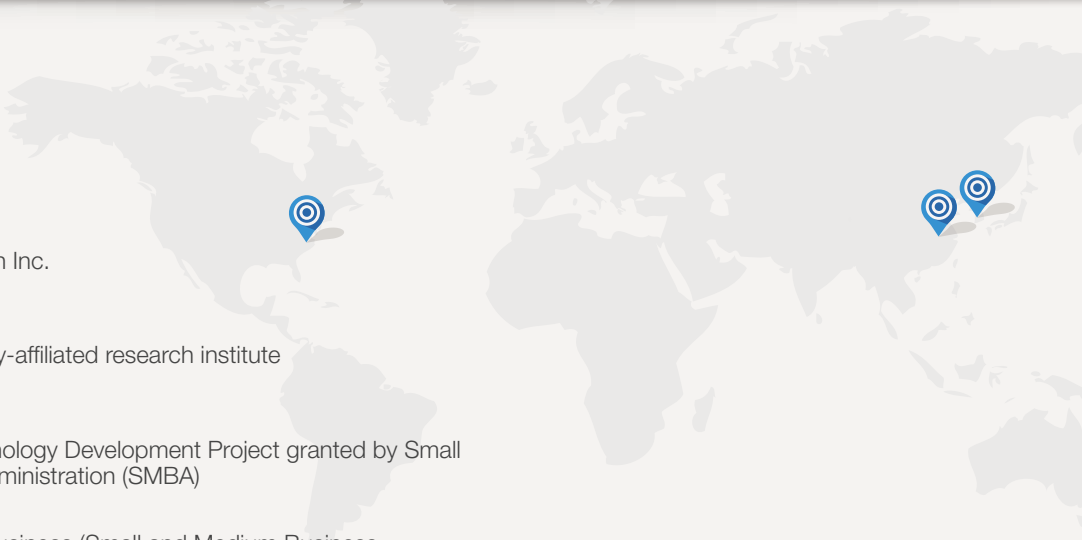
Property	Value	Unit
Absolute Entropy of Ideal Gas at 298.15K and 1bar	63.7624	cal/mol/K
Acentric Factor	0.248832	dimensionless
Critical Compressibility Factor	0.274652	dimensionless

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)
  - 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
  - Received foreign direct investment from China
  - 2012** Registered trademark of ChemEssen for Domestic/Overseas
  - 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
  - Launched Mol-Instincts Web Search (web version)
  - 2015** Updated Mol-Instincts DB with over 2.7million compounds / Cooperation with the Korea University (CHERIC)
  - Launched Real Time Predictor
  - 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>

 **MOL-Instincts**



[www.ChemEssen.com](http://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.

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