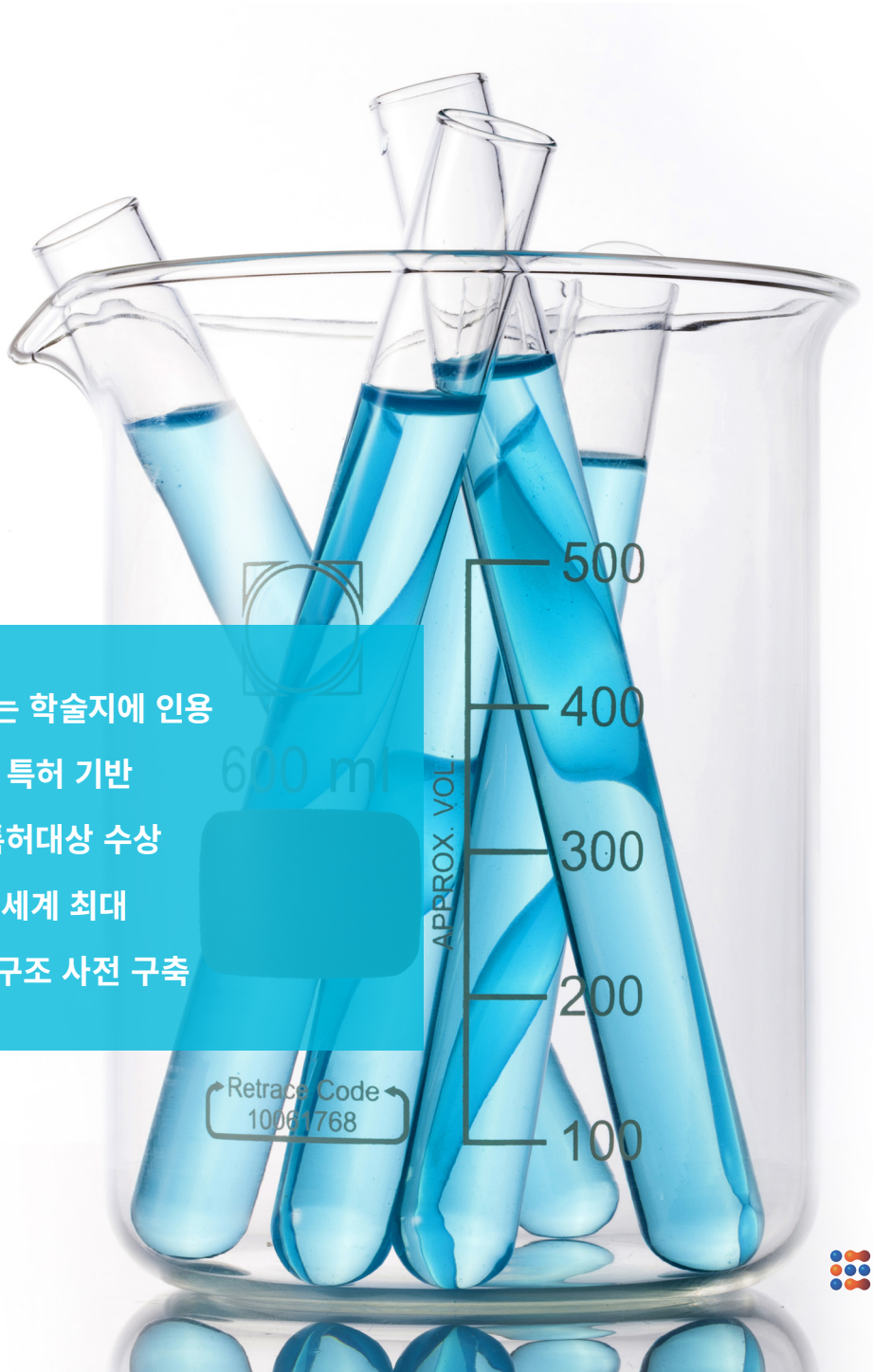
MOL Instincts

화학물질정보 데이터베이스 소개서

Mol-Instincts

세계최대의 화학물질정보 데이터베이스는 대한민국에 있습니다.



네이처 등 권위있는 학술지에 인용

등록 완료된 41개 특허 기반

2014 대한민국 특허대상 수상

화학 정보량 기준 세계 최대

네이버 화학물질 구조 사전 구축

ChemEssen

What is **Mol-Instincts**?

네이처 등 권위있는 학술지에 인용

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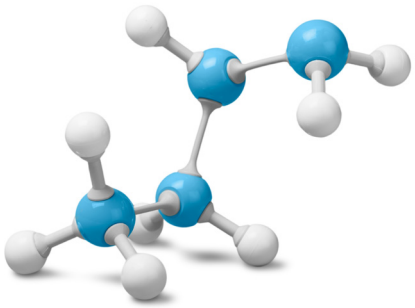


NEW

화학물질정보 데이터베이스

Mol-Instincts는 양자화학 기반으로 구축된 세계최초의 화학물질 정보 데이터베이스입니다.

400만개

이상의 화학물질과 약 80억 개의 정보 수록

화합물질 1개당 2,100개 이상의 물성 정보를 포함하고 있습니다.

95%

이상의 예측정확도

Mol-Instincts의 물성 예측값을 현존하는 실험값과 비교하였을 때, 대부분 95% 이상의 정확도를 보였습니다.

(기존 예측방법인 Joback Method의 끓는점 정확도는 63% 정도임)

주요 화학물질

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+

제공정보 및 응용분야

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)

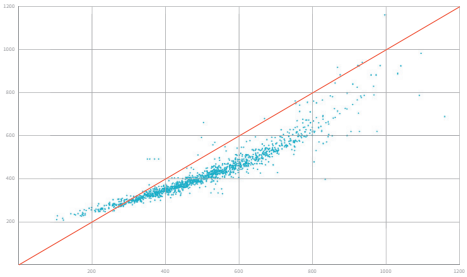
개발 프로세스

(관련 특허 40건 취득)

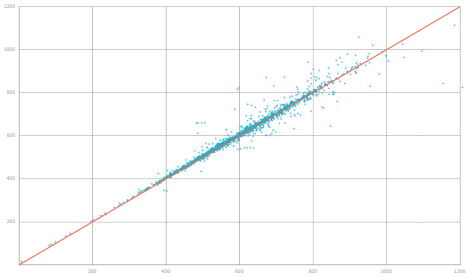
Mol-Instincts Development Process

STEP 1	**High Quality Quantum Calculation**	Conformer structure를 분석하여 가장 안정한 구조를 양자화학 계산의 초기 구조로 사용
STEP 2	**Most Advanced QSPR Modeling**	양자화학 결과를 포함한 2,000가지 이상의 molecular descriptor를 기반으로 최적의 QSPR모델 구축
STEP 3	**Detailed Model Verification**	현존하는 대부분의 실험값(7년이상 수집)과 예측값을 비교하여 정확도가 95% 이상임을 검증
STEP 4	**Chemical Property Categorization**	다양한 종류의 화합물과 화합물 당 2,100가지 정보를 수록하는 DB 개발 완료

기존 기술의 예측정확도(Joback방법): 63.07%



Mol-Instincts의 예측정확도: 95.02%



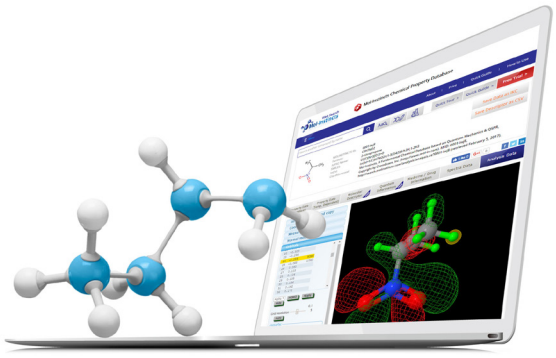
Mol-Instincts는
네이처 등 권위있는 학술지에
다수 인용되고 있습니다.

하기는 일부 발췌된 목록입니다.

PUBLISHER	PUBLICATION
NATURE	Fractal Based Analysis of the Inflence of Odorants on Heart Activity. Hamidreza Namazi, Vladimir V. Kulish. Scientifi Reports 6, Article number: 38555, DOI:10.1038/srep38555 (2016)
NATURE	The Analysis of the Inflence of Odorant's Complexity on Fractal Dynamics of Human Respiration. Hamidreza Namazi, Amin Akrami,Vladimir V. Kulish. Scientifi Reports 6, Article number: 26948, DOI:10.1038/srep26948 (2016)
NATURE	Gold Nanoparticle Monolayers from Sequential Interfacial Ligand Exchange and Migration in a Three-Phase System. Guang Yang, T.Hallinan. Scientifi Reports volume 6, Article number: 35339, DOI:10.1038/srep35339 (2016)
American Chemical Society (ACS)	Propylphenol to Phenol and Propylene over Acidic Zeolites: Role of Shape Selectivity and Presence of Steam. Yuhe Liao, Ruyi Zhong, Ekaterina Makshina, Martin d'Halluin, Yannick van Limbergen, Danny Verboekend, and Bert F. Sels. ACS Catal. 2018, 8, 7861-7878, DOI:10.1021/acscatal.8b01564(2018)
American Chemical Society (ACS)	Role of Ligand Straining in Complexation of Eu3+–Am3+ Ions by TPEN and PPDEN, Scalar Relativistic DFT Exploration in Conjunction with COSMO-RS. Sk. Musharaf Ali. ACS Omega 2018, 3, 13104-13116, DOI: 10.1021/acsomega.8b00933 (2018)
American Chemical Society (ACS)	Extension of the SAFT-VR Mie EoS To Model Homonuclear Rings and Its Parametrization Based on the Principle of Corresponding States. Erich A. Müller, Andrés Mejía. Langmuir, 2017, 33 (42), pp 11518–11529, DOI: 10.1021/acs.langmuir.7b00976 (2017)
American Chemical Society (ACS)	Calculation of Average Molecular Parameters, Functional Groups, and a Surrogate Molecule for Heavy Fuel Oils Using 1H and 13C Nuclear Magnetic Resonance Spectroscopy. Abdul Gani Abdul Jameel, Ayman M. Elbaz, Abdul-Hamid Emwas, William L. Roberts, S. Mani Sarathy. Energy Fuels, 2016, 30 (5), pp 3894–3905, DOI: 10.1021/acs.energyfuels.6b00303 (2016)
American Chemical Society (ACS)	Comparative Study of the Ignition of 1-Decene, trans-5-Decene, and n-Decane: Constant-Volume Spray and Shock-Tube Experiments. Aniket Tekawade, Tianbo Xie, Matthew A. Oehlschlaeger. Energy Fuels, 2017, 31 (6), pp 6493–6500, DOI: 10.1021/acs.energyfuels.7b00430 (2017)
American Chemical Society (ACS)	Computing the Diamagnetic Susceptibility and Diamagnetic Anisotropy of Membrane Proteins from Structural Subunits. Mahnoush Babaei, Isaac C. Jones, Kaushik Dayal, Meagan S. Mauter. J. Chem. Theory Comput., 2017, 13 (6), pp 2945–2953, DOI: 10.1021/acs.jctc.6b01251 (2017)
ELSEVIER	SGC based prediction of the flash point temperature of pure compounds. Tareq A. Albahri, Norah A.M. Esmael. Journal of Loss Prevention in the Process Industries 54, July 2018, Pages 303-311, DOI: 10.1016/j.jlp.2018.05.005 (2018)
ELSEVIER	Shape selectivity vapor-phase conversion of lignin-derived 4-ethylphenol to phenol and ethylene over acidic aluminosilicates: Impact of acid properties and pore constraint. Yuhe Liao, Martin d'Halluin, Ekaterina Makshina, Danny Verboekend, Bert F.Sels. Applied Catalysis B: Environmental. 234, 15 October 2018, Pages 117-129, DOI: 10.1016/j.apcatb.2018.04.001 (2018)
ELSEVIER	Spontaneous motion of various oil droplets in aqueous solution of trimethyl alkyl ammonium with diffrent carbon chain lengths. Ben Nanzai, Megumi Kato, Manabu Igawa. Colloids and Surfaces A: Physicochemical and Engineering Aspects, Volume 504, 5 September 2016, Pages 154-160, DOI: 10.1016/j.colsurfa.2016.04.063 (2016)
ELSEVIER	Electron scattering from C2-C8 symmetric ether molecules. Paresh Modak, Suvam Singh, Jaspreet Kaur, Bobby Antony. International Journal of Mass Spectrometry, 2016, Volume 409, Pages 1-8, DOI: 10.1016/j.ijms.2016.09.002 (2016)
Oxford Academic	Plant Cuttings. Nigel Chaffey. Annals of Botany, Volume 121, Issue 6, 11 May 2018, Pages iv–vii, DOI: 10.1093/aob/mcy070 (2018)
Royal Society of Chemistry (RSC)	Physical Chemistry of Energy Conversion in Self-propelled Droplets Induced by Dewetting Effect. B. NANZAI, T. BAN. In: Self-organized Motion: Physicochemical Design based on Nonlinear Dynamics, 2018 (2018)
Royal Society of Chemistry (RSC)	"Nitrile-assistant eutectic electrolytes for cryogenic operation of lithium ion batteries at fast charges and discharges. Yoon-Gyo Cho, Young-Soo Kim, Dong-Gil Sung, Myung-Su Seo, Hyun-Kon Song. Energy Environ. Sci., 2014,7, 1737-1743 DOI: 10.1039/C3EE43029D (2014)"
Springer	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Antony J. Williams, Christopher M. Grulke, Jeff Edwards, Andrew D. McEachran, Kamel Mansouri, Nancy C. Baker, Grace Patlewicz, Imran Shah, John F. Wambaugh, Richard S. Judson, Ann M. Richard. J Cheminform (2017) 9:61, DOI: 10.1186/s13321-017-0247-6 (2017)
Springer	Multi-agent System for Forecasting Based on Modified Algorithms of Swarm Intelligence and Immune Network Modeling. Samigulina G.A., Massimkanova Z.A. In: Agents and Multi-Agent Systems: Technologies and Applications 2018. Jezic G., Chen-Burger YH., Howlett R., Jain L., Vlacic L., perka R. (eds) KES-AMSTA-18 2018. Smart Innovation, Systems and Technologies, vol 96. Springer, Cham (2018)
Springer	Electron-Transfer Secondary Reaction Matrices for MALDI MS Analysis of Bacteriochlorophyll a in Rhodobacter sphaeroides and Its Zinc and Copper Analogue Pigments. Calvano CD, Ventura G, Trotta M, Bianco G, Cataldi TR, Palmisano F. J Am Soc Mass Spectrom. 2017 Jan, 28(1), 125-135. DOI: 10.1007/s13361-016-1514-x (2017)
Springer	A modified scaled variable reduced coordinate (SVRC)-quantitative structure property relationship (QSPR) model for predicting liquid viscosity of pure organic compounds. Seongmin Lee, Kiho Park, Yunkyung Kwon, Dae Ryook Yang. Korean Journal of Chemical Engineering, 2017, 34, 2715-2724, DOI: 10.1007/s11814-017-0173-3 (2017)
Springer	Many InChIs and quite some feat. Wendy A. Warr.Journal of Computer-Aided Molecular Design, 2015, Volume 29, Issue 8, pp 681–694, DOI: 10.1007/s10822-015-9854-3 (2015)
Taylor & Francis	Microbial growth yield estimates from thermodynamics and its importance for degradation of pesticides and formation of biogenic non-extractable residues. A. L. Brock, M. Kästner, S. Trapp. SAR and QSAR in Environmental Research, Volume 28, 2017, DOI: 10.1080/1062936X.2017.1365762 (2017)

사용방법

How To Use Mol-Instincts



①	Mol-Instincts 검색 웹사이트 접속	http://search.molinstincts.com
②	Text / Structure 중 원하는 방법으로 **화합물 검색**	Search a Compound
③	일치하는 화합물의 '**View our data**' 클릭한 후 물성 뷰페이지로 이동	View our data
④	**유사 화합물**도 함께 조회할 수 있으며 일치율도 함께 표시됨	Results with Matching Accuracy
⑤	7가지 카테고리의 물성 특성별 탭에서 원하는 **물성 확인**	View Chemical Properties

켐에쎈은 **화학**과 **정보 기술**의 융합을 통한
새로운 솔루션을 제공하고있습니다.

CONTACT US

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