

“ I need to know
the structure of
this compound ”

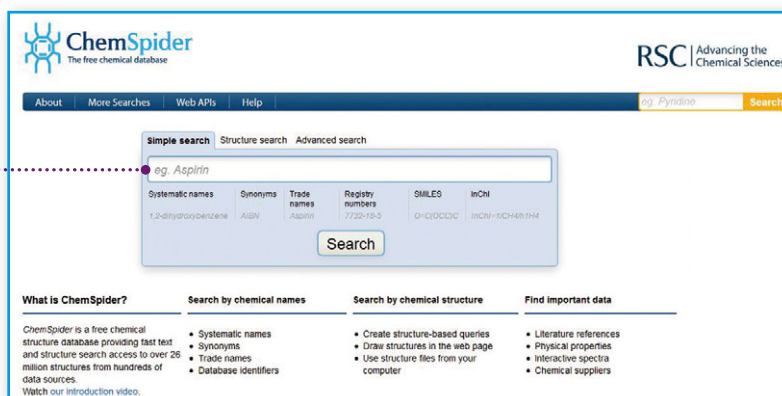
ChemSpider can help you!

We know that chemical naming is hard and that trivial names hide complex structures.

We want to make it easy for you to find this information wherever you are:

• In the lab • At home • At a conference

A simple and intuitive
text search.



What is ChemSpider?
ChemSpider is a free chemical structure database providing fast text and structure search access to over 26 million structures from hundreds of data sources.
Watch our introduction video.

Search by chemical names

- Systematic names
- Synonyms
- Trade names
- Database identifiers

Search by chemical structure

- Create structure-based queries
- Draw structures in the web page
- Use structure files from your computer

Find important data

- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers

Once you've found a structure,
save it in a format that can be
opened in any chemical
drawing program; use it again
and again.



Search term: **brevetoxin B** (Found by approved synonym)

Brevetoxin B

ChemSpider ID: **9041149**

Molecular Formula: $C_{50}H_{70}O_{14}$

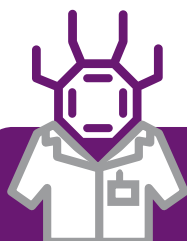
Average mass: 895.08197 Da

Monoisotopic mass: 894.47699 Da

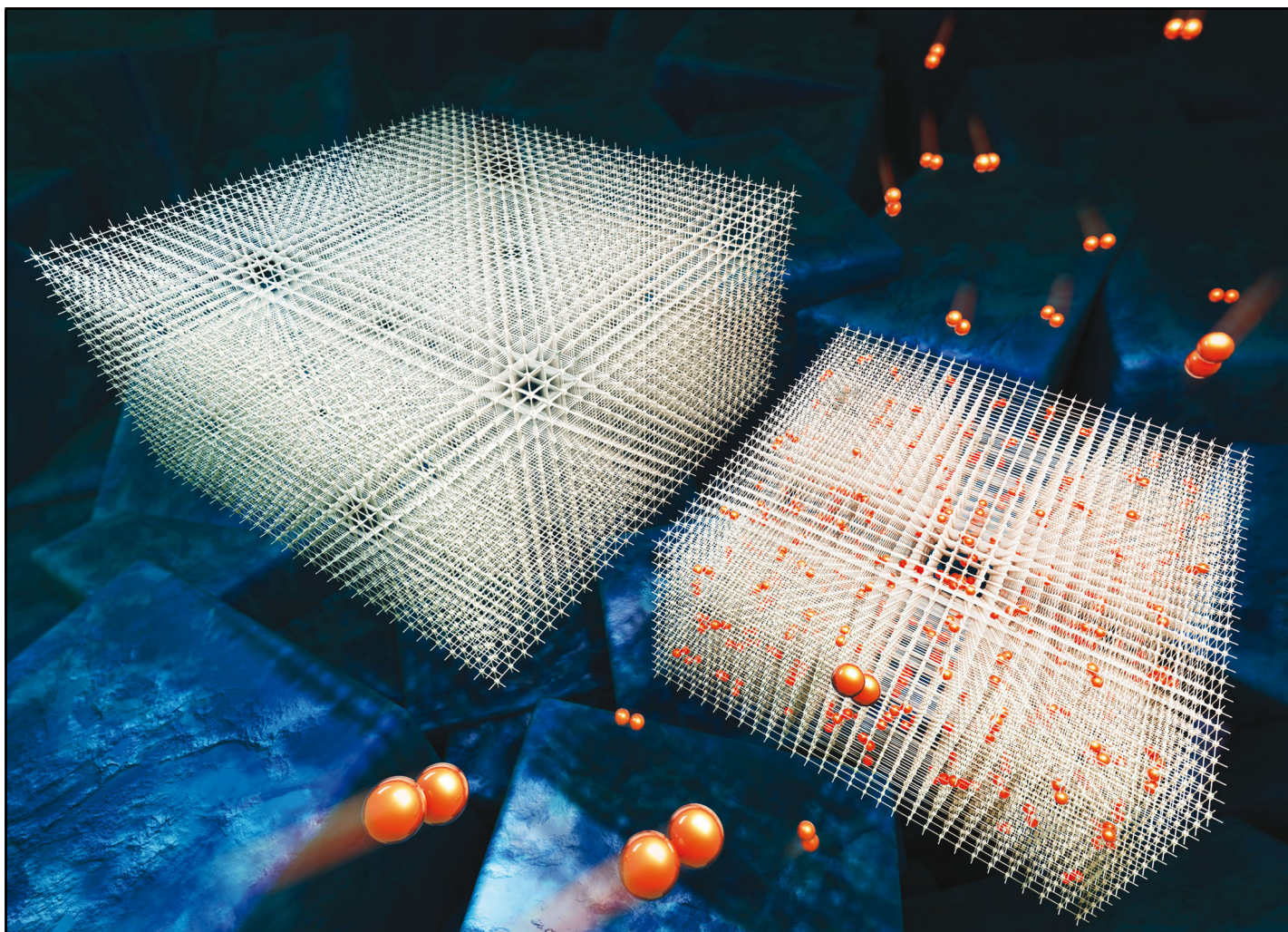
Systematic name

2-[[[(1S,3R,4aR,5aS,6aR,7Z,9aS,10aR,11aS,12aR,13R,14aS,15aR,16aS,20aR,21aS,22aR,23aS,25aR,26aS,27aR,28aS,29aR,30aS)-1-Hydroxy-9a,13,20,21a,25a,26a,30a-heptamethyl-18-oxo-2,3,4a,5,5a,6a,9,9a,10a,11,11a,12a,13,14,14a,15a,16,16a,18,20a,21a,22,22a,23a,24,25,25a,26a,27,27a,28a,29,29a,30a-tetratricontahydro-1H-pyrano[2',3'':5',6'']pyrano[2'',3''':5'',6''']pyrano[2''',3''':6'',7'']oxepino[2'',3''':6'',7'']oxepino[2'',3''':5'',6'']pyrano[2',3':5,6]pyrano[2,3-g]oxocin-3-yl)methyl]acrylaldehyde

View the image in 3D.



And remember, **ChemSpider** gives you access to a database containing 28 million chemical structures and all of this information: **FREE**, for **Anyone**, **Anytime**, **Anywhere**



Showcasing research work from the research group of Dr Sang Soo Han, Korea Institute of Science and Technology.

Title: Volume shrinkage of a metal-organic framework host induced by the dispersive attraction of guest gas molecule

An extraordinary metal-organic framework (MOF) phenomenon has been newly discovered. Adsorption of hydrogen molecules in MOF-5 leads to volume shrinkage, which is in contrast to the intuitive notion that gas adsorption in a confined system leads to volume expansion.

As featured in:



See Kim, Han *et al.*,
Phys. Chem. Chem. Phys.,
2013, **15**, 18822.

www.rsc.org/pccp

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