

“ I need to know  
the structure of  
this compound ”

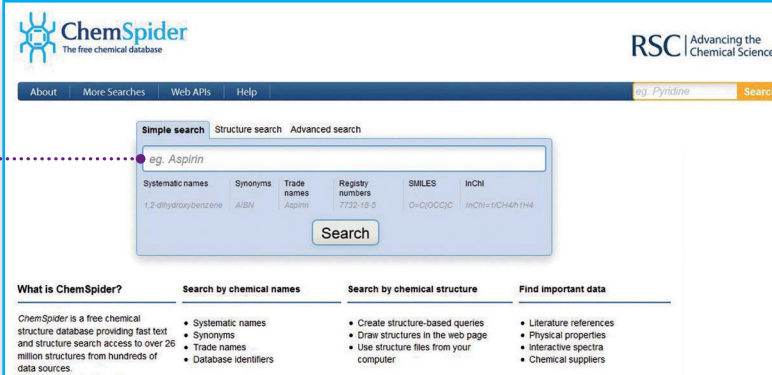
## ChemSpider can help you!

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.



The screenshot shows the ChemSpider homepage with a search bar containing "eg. Aspirin". Below the search bar, a table displays search results for Aspirin:

Systematic names	Synonyms	Trade names	Registry numbers	SMILES	InChI
1,2-dihydroxybenzene	ASPN	Aspirin	7732-18-5	O=C(O)CC(=O)C	OC(=O)C1=CC=CC=C1

Below the table is a "Search" button. At the bottom of the page, there are sections for "What is ChemSpider?", "Search by chemical names", "Search by chemical structure", and "Find important data".

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.



The screenshot shows the search results for "brevetoxin B". The search term is "brevetoxin B (Found by approved synonym)". The structure is displayed as a 3D ball-and-stick model. To the right of the structure, the following information is provided:

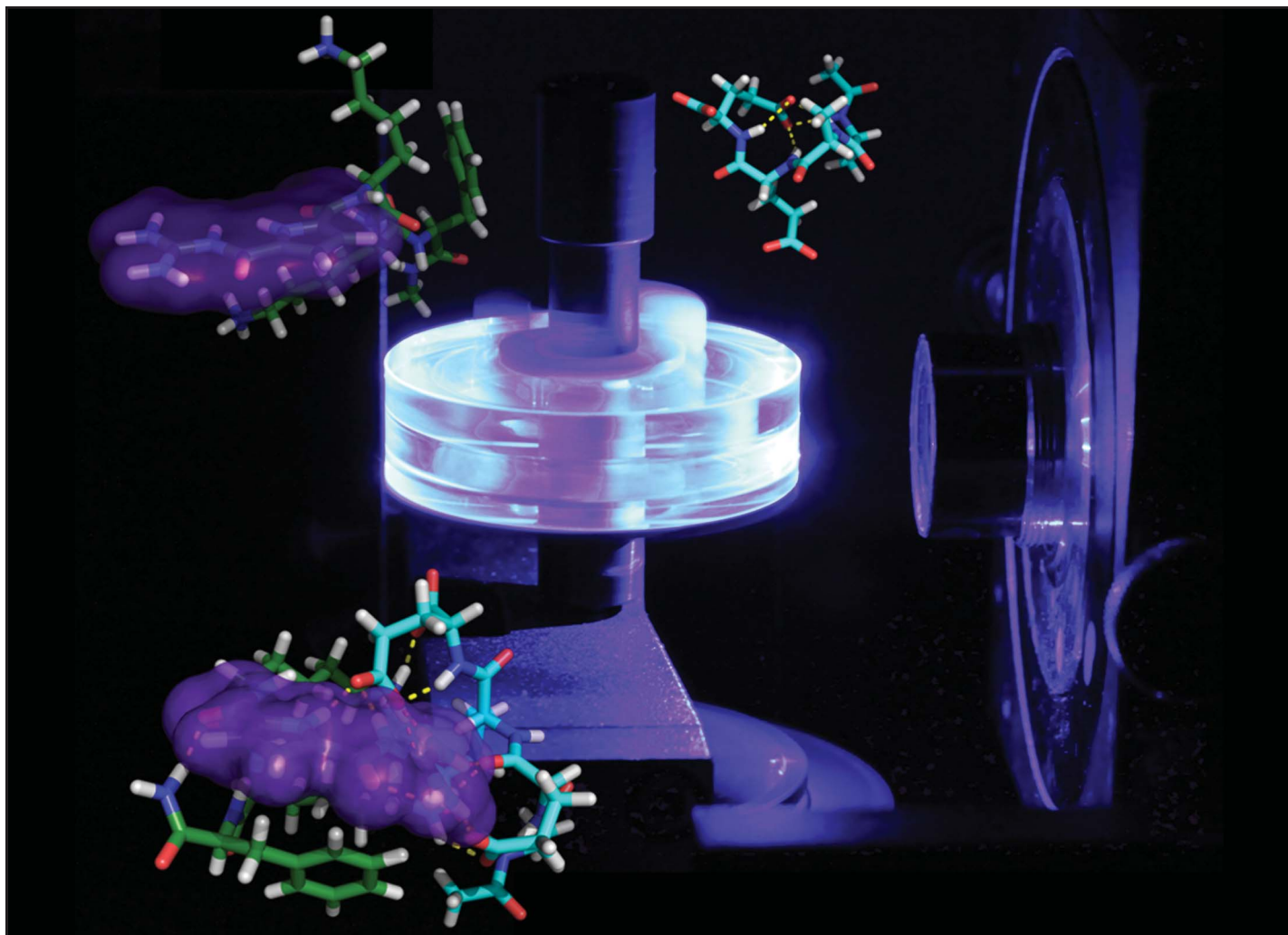
**Brevetoxin B**  
 ChemSpider ID: 9041149  
 Molecular Formula: C<sub>60</sub>H<sub>70</sub>O<sub>14</sub>  
 Average mass: 895.08197 Da  
 Monoisotopic mass: 894.47699 Da

Below this information is a section for the "Systematic name" which is a long, complex IUPAC name. At the bottom of the structure, there are buttons for "Cell 2D 3D Save Zoom" and a note "23 of 23 defined stereocentres".

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**

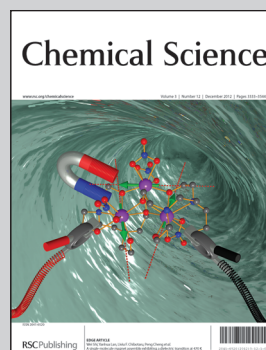


Showcasing research from Professor Sebastian Schlücker's Laboratory, Department of Physics, University of Osnabrück, Germany.

**Quantitative label-free monitoring of peptide recognition by artificial receptors: a comparative FT-IR and UV resonance Raman spectroscopic study**

The combination of Raman and IR spectroscopy with multivariate analysis is an emerging approach for quantitative label-free monitoring of molecular recognition processes, e.g. between tetrapeptides and an artificial receptor.

**As featured in:**



See Sebastian Schlücker *et al.*, *Chem. Sci.*, 2012, **3**, 3371.

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