

ChemSpider

Secure Access

With ChemSpider Secure Access, the data you're searching for is at your fingertips...



ChemSpider provides fast access to over 30+ million structures, properties and associated information. By integrating and linking compounds from over 500 data sources, ChemSpider enables researchers to discover the most comprehensive view of chemical data from a single online search. Making it the perfect place for researchers to start their chemistry search...

ChemSpider grows daily with more depositions and more links provided by researchers from around the world invited to build and curate this data.

ChemSpider is being used Commercially by a variety of global chemical and pharmaceutical companies.

Web Services

Why choose ChemSpider for your researchers?

- Fast access via API (application programme interface)
- Always evolving data grows daily
- Award winning everyone is talking about it
- Community driven be part of advancing a resource for the chemistry community across the globe
- Customised Solutions prices and data models are flexible based on your specific needs

Key benefits & insights

- Quick and easy to use, web services link with your own software ensuring high volume usage is supported
- Real time searches, ChemSpider is growing daily, get the most up-to-date results

Sub-Licensing

Purchase the data in full and gain the rights to sell the data onto licenced users. Pricing is based on tiers of usage per annum.

The Simple Set

We will provide you with:

- Generation of SMILES from a chemical structure
- Generation of a chemical structure from SMILES
- Generation of an InChI from a chemical structure
- Generation of a chemical structure from an InChl
- Conversion between chemical data formats
- Retrieving chemical structure thumbnail

The Advanced Set

Includes the Simple Set and the following:

- Search by chemical identifier
- Search by structure or substructure
- Search by molecular mass or elemental composition
- Search by predicted properties
- Retrieving data source links

For large organisations; usually multinational users. Pricing is based on tiers of usage per annum.

ChemSpider Dataset

Purchase the data in bulk for integration within your internal system. Contact your ChemSpider sales representative for more information.

Key benefits & insights

- We guarantee secure access with no compromise
- Quarterly updates available ensuring you stay up-to-date with the latest data

Structure Dataset

Offers all the current molecular structures on ChemSpider. Focus is structural data only: the structures, SMILES and InChI nomenclature, as a structure-data file (SDF).

 Provided on a USB stick, disk or via FTP.

Dataset prices per sub-licenced customer

Price is based on the number of users in an organisation and the number of structures/validated names. Data is provided once – no updates.





Includes the Structural Datasets and also includes the list of validated names/synonyms/common names.

 Provided on a USB stick, disk or via FTP.





Spectral Dataset

Includes all of the spectral data and associated chemical compounds within the ChemSpider data repository.

No data links included

 Provided on a USB stick, disk or via FTP.

Secure Socket Layer (SSL)

What is included?

Encrypted search solution with secure access to ChemSpider web services. When you search using SSL, your search queries and traffic are encrypted. This means that intermediary users that might have access to your network can't see your results and search terms. We will provide a signed legal document detailing that information regarding search items (such as logs) will remain confidential.

What happens?

- We will send you a monthly report, detailing IP addresses and the usage levels of those IP addresses.
- A list of designated IP Addresses (supplied by your organisation) will go through the secure access set up by us.



ChemSpider Secure Access

We understand the privacy issues around confidential access to chemical data. We are currently partnering with global Pharmaceutical organisations, providing secure access to ChemSpider data.

Key benefits & insights

- Trial access will be provided for 1 month
- Available for unlimited number of sites

Please get in touch to see how we can help support you and your research needs.

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