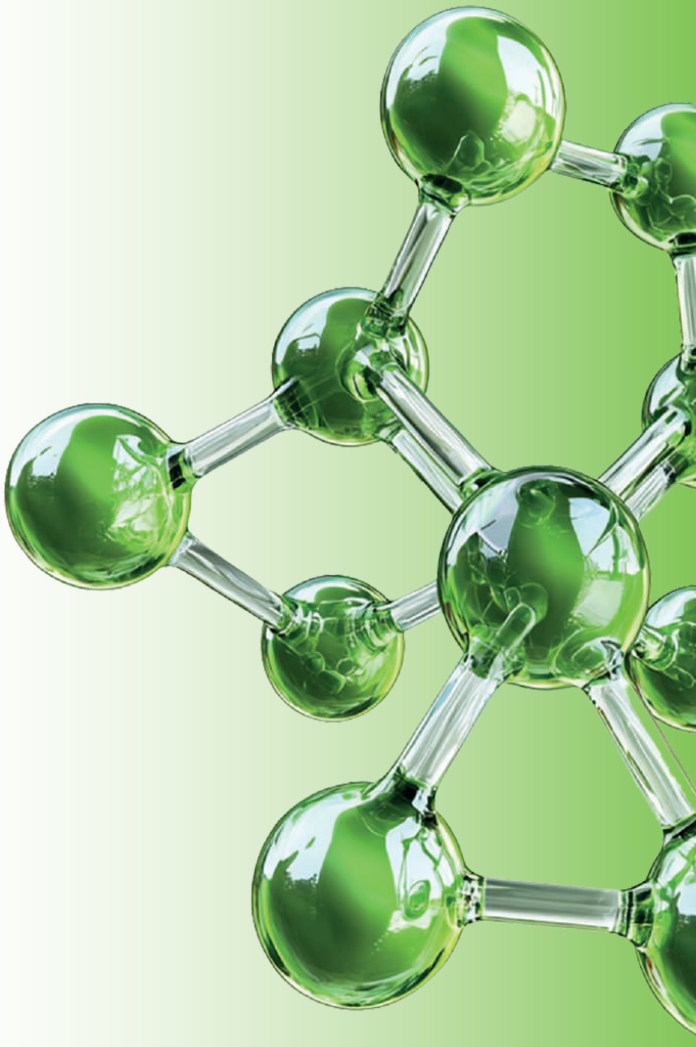

CHEMSPACE
Delivering Discovery Solutions®

YOUR GLOBAL PROVIDER OF DRUG DISCOVERY SERVICES

WHO WE ARE?

Chemspace is a global partner in drug discovery, enhancing hit finding with advanced Computational Chemistry, Bioinformatics, and Machine Learning tools. By exploring ultra-large chemical spaces, we deliver high-quality hit molecules for discovery projects. With access to the largest online catalog of over 13 billion molecules, you can efficiently find the compounds you need.

Looking for an end-to-end solution? Our integrated projects combine hit identification services with biological validation, providing a seamless path from early-stage discovery to pre-clinical studies.

Olga Tarkhanova, PhD. CEO at Chemspace LLC

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150+
WORLDWIDE SUPPLIERS

SALES GEOGRAPHY
80+
COUNTRIES

US AND EU
SHIPPING HUBS

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DRUG DISCOVERY SERVICES

EFFICIENT HIT FINDING

- DNA-encoded libraries with ML-supervised data processing
- Giga-scale virtual screening (V-SYNTHES)
- Fragment-based Drug Discovery
- ML-boosted giga-scale docking
- Virtual screening
- Molecular dynamics simulation
- SAR by catalog, 2D/3D QSAR
- Machine Learning-based services
- Generative AI
- HTS-ML

INTEGRATED DRUG DISCOVERY

HIT IDENTIFICATION

Assay development
(cell-based, biochemical, biophysical)
HTS
Fragment screening
DEL-ML-CS
Crystallography screening
Giga-scale ML-assisted virtual screening

HIT-TO-LEAD

Computer-aided drug design
Generative AI
Custom library design and synthesis
Scaffold decoration
Selectivity (off-target activity)
ADME profiling
In vitro and in vivo DMPK

PRECLINICAL STUDIES

Safety profiling
Receptor profiling
Ligand binding
Additional in vitro
and in vivo characterization
Synthetic optimization
of candidates
Metabolic and impurity identification synthesis

TARGET ANALYSIS AND DRUGGABILITY ASSESSMENT

Molecular biology
Cell lines
Protein production
Structure-based assessment
Allosteric sites prediction
PPI modulation

HIT EXPANSION, SAR BY CATALOG

ML-assited SAR
2D/3D QSAR
Custom space generation
Scaffold hopping
3D pharmacophore similarity
Steered MD/mmPBSA
ADME/Tox predictions

LEAD OPTIMIZATION

Medicinal chemistry support
Custom library design and synthesis
Custom synthesis
ADME profiling
In vitro and in vivo DMPK
Acelerated DMTA cycle

CATALOG

13B	small molecules
880K	antibodies, peptides, and proteins
142B	Freedom space compounds
70B	REAL space compounds
65	compound sets & pre-plated libraries
1400	AI-supported focused libraries

PURCHASING SOFTWARE AS A SERVICE

Focus on your research while we will handle the rest!

PUNCHOUT SITE

Our Punchout integration allows you to access the Chemspace catalog directly from your ERP system. You can search, browse for compounds, and add items to your cart within the Punchout site. Once ready, you cart details are transferred back to your ERP by checkout botton, where you can finalize and place the order through your standard procurement process.

CUSTOM PLATFORM

Custom platform is a web-based portal developed on the prototype of the Chemspace website, customizable with features tailored to your specific needs. Unlike a Punchout Site, a Custom Platform operates independently of the client's procurement system while seamlessly covering all steps of the ordering process, from compound search to order delivery.

CHEMSPACE API

Chemspace API is your gateway to our entire database. Whether you are searching for specific chemical structures or by identifiers, the API has you covered. Chemspace API provides access to public database: structure searches (exact match, substructure search, similarity search), text searches, as well as lead time and price of the compounds.

FEATURES & FUNCTIONALITY

SEARCH

Search in 13+ billion compounds using exact match, substructure, and similarity search options.

REQUEST

Request items that are either not listed in our catalog or currently unavailable.

ORDER

Submit the order in your procurement system after check out from the Pucnhout site or custom platform.

UPDATES

Get electronic notifictions about your synthesis & order shipping status.

RECEIVE

Receive your order on multiaddress.

GET INVOICED

Receive electronic invoices through ERP system and make payment.

COMPOUND MANAGEMENT

SDS TOOLS

- Assigning process of compound passport
- Assigning HTS code for all compounds
- Transport class assignment to all compounds
- Customizable SDS

STORAGE

- Storage space and facilities in the USA and EU
- Ambient temperature
- Cold room (-20°C)
- Refrigerators (-40°C)

REFORMATTING

- Reweighing, relabeling, dissolution
- Automated multi-format plating and reformatting
- Using a wide range of labware on customer's demand
- Dose response curve (DRC)
- Cherry-picking

DATA MANAGEMENT

- Personalized support
- Real-time inventory tracking
- Automated order processing
- User access control
- Compatibility with lab systems

QUALITY CONTROL

- Verification of incoming compounds
- Barcode & database entry
- Spectral data (LC/MS, HRMS, NMR)
- Regular retesting & stability checks
- Validate labeling accuracy

LOGISTIC AND SHIPPING

- Shipments with ice pack or dry ice
- Customs clearance support
- Multiple shipments to different sites
- Consolidated shipment and dropship
- Worldwide delivery couriers

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