

Chemspace Catalog Data Format

Field Name	Requirement	Field Type	Comment
STRUCTURE	Mandatory	Text	Chemical structure denoted as SMILES string or as MOL (V2000 or V3000) text block when the catalog is submitted in SDF format. It is highly recommended to make sure that chiral flag within MOL-block is properly set if your submission contains structures with both absolute and relative stereochemical configuration. For correct representation of more complex structural features please use SDF with MOL V3000 format.
Vendor_Item	Mandatory	Text	A unique identifier for your product. Never reuse item numbers of discontinued products to reference any other product. If you normally identify unique structure, you may append pack size (for example) to your structure identifier (Structure_Cat_Number) to obtain valid Vendor_Item value.
Pack_size	Mandatory	Decimal	For example: 2.75
Pack_unit	Mandatory	Text	Mass or volume unit. Allowed values are: KG, G, MG, L, ML.
Purity	Mandatory	Decimal	For example: 99.99. Never put extra symbols in this field, like ">", "+", "%" etc.
Delivery_time	Mandatory	Integer	Number of days required to deliver the item
In_stock	Mandatory	Binary	Allowed values: 1 – item maintained in stock, 0 – made to order item
Density	Conditional	Decimal	Value in "g/ml" must be provided if pack unit references volume.
Structure_Cat_Number	Optional	Text	A unique identifier for the chemical structure in your catalog.
CAS	Optional	Text	Strictly one CAS number per structure.
MFCID	Optional	Text	Strictly one MFCID-number per structure.
Chemical_name	Optional	Text	Chemical name – please do not include additional information here, provide it in the 'Description' field as needed.
H_code	Optional	Text	List of semicolon-separated H-codes according to GHS classification.
H_category	Conditional	Text	List of semicolon-separated hazard categories corresponding to H-codes (please preserve the order). Hazard categories have to be specified for all records containing H-codes which may be attributed ambiguously.
Price_USD	Optional	Decimal	Price in USD. Items without price will be considered POA.
Price_EUR	Optional	Decimal	Price in EUR. Items without price will be considered POA.
Price_CHF	Optional	Decimal	Price in CHF. Items without price will be considered POA.
Price_GBP	Optional	Decimal	Price in GBP. Items without price will be considered POA.
Storage_conditions	Optional	Text	Allowed values are: Cold, Cool, Freezer, Controlled Cold Temperature, Room Temperature, Controlled Room Temperature, Dry Place.
Transport_conditions	Optional	Text	Allowed values are: Cold, Cool, Freezer, Controlled Cold Temperature, Room Temperature, Controlled Room Temperature, Dry Place.
UN_number	Optional	Text	UN number (also called UN ID) for hazardous items.
WGK	Optional	Integer	German water hazard class. Allowed values: 1, 2, 3.

Controlled_substance	Optional	Text	List of comma-separated ISO country codes where the substance is under special control (like DEA Lists, etc.)
Product_URL	Optional	Text	URL to product in supplier's own electronic catalog (starting from http:// or https://). Never include extra text like e-mail or comments here.
Description	Optional	Text	Briefly describe any important details about your product not listed elsewhere within catalog record, for example: "1M cyclohexane solution", "stabilized with p-Methoxyphenol", "enantiomeric excess 85%", etc. This information will be appended to the chemical name, purity and pack size.

Catalog preparation notes for automated submission through Personal cabinet (My Space).

Field names in submitted file must precisely match specification. Values from unmatched fields will be ignored. Absence of a valid value in a mandatory field prevents record from being accepted.

Allowed catalog file formats are: SDF, tab-separated plain text. In case of plain text file first line must contain field headers, escape characters should not be used throughout the file. File may be zipped to facilitate upload. Do not put multiple files in a zip archive. Password protected zip archives will not be processed.

Please refrain from including in your submission products which clearly cannot be used as organic chemical building blocks, i.e. bulk inorganic chemicals, food additives, surfactants, polypeptides, ion-exchanging resins etc. Submitted structures have to be uncharged. If you believe that particular product has to be included but it fails structure validation, please contact our technical support and your case will be evaluated by our data management team.

It is advantageous to provide prices in multiple supported currencies as it improves impression of your catalog items by prospective buyers.

Catalog update modes

“Add new items” All validated records from the submitted file will be added to the catalog. Records existing in the catalog (if any) will not be modified.

“Update items” Only records in the current catalog with matching Vendor_Item values will be updated. Unmatched records from the submitted file will not be added. Vendor_Item is the only mandatory field in the submitted file for this mode. Attribution of items to Chemspace structures cannot be changed in this mode. If previously submitted optional value needs to be removed, please use reserved value “n/a” in the corresponding field.

“Delete items” Items with matching Vendor_Item values will be removed from the catalog. Please submit plain text file with one Vendor_Item value per line and no other data.

“Full update” Completely replace all records in the current catalog with validated records from the submitted file. This mode is equivalent to combination of “Delete items” for all existing catalog records followed by “Add new items” on an emptied catalog.

Catalog submission consists of the following steps *:

- 1) the file is uploaded or fetched from the URL as specified by the user and automatically placed in processing queue;
- 2) the file is analyzed to validate its contents, validation log is generated – this step may take substantial time depending on the number of items in your catalog and processing queue length;
- 3) all validated records are made available for publication – the user needs to confirm (or cancel) publication from the personal cabinet;
- 4) if the publication was confirmed, then validated records are queued for publication and are published automatically.

* in “item deletion” update mode there are no validation/publication stages, all matching items are removed from the catalog instantaneously.

The validation log generated on step 2 may contain important information about submitted items, therefore it is highly recommended to examine the validation log before proceeding to step 3.

While catalog update is being processed, no other activity influencing catalog records for a given supplier can be performed, except for queuing submission files for other existing catalogs (if any).