**MolPort Chemical Search**

**API v.3.0.**

11.10.2015

Revision

|  |  |  |  |
| --- | --- | --- | --- |
| **Version** | **Date** | **Author** | **Description** |
| 1.0 | 30-07-2015 | Normunds Kinne | Initial draft |

##

Response structure

*MolPort JSON* response generic form is:

{

 "Result": {

 "Status": 1|2,

 "Message": <message text>

 },

 "Data": {

 "Version": <version number>,

 … <Data Object> …

 }

}

where:

Status – int; possible values:

1 – operation successful,

2 – operation was not successful;

Message – string; short informative, human readable message;

Version – string; version number of returned *MolPort JSON* data objects;

Data Object – json; *JSON* representation of returned data objects.

API Methods

## Load molecule

Method to load information about molecule from *MolPort* database if *MolPort ID* is known.

## Request

|  |  |
| --- | --- |
| **Method** | **URL**  |
| **GET** | /api/molecule/load/{molecule id} |
| **JSON** | None |

## Example

|  |  |
| --- | --- |
| **Method** | **URL**  |
| **GET** | http://www.molport.com/api/molecule/load/2325020 |

## Response

Method will return a Molecule object with data structure:

Id – int; molecule identifier in *MolPort* database;

MolPort Id – string, formatted molecule identifier in *MolPort* database;

SMILES – string; *SMILES* of molecule;

IUPAC – string; *IUPAC* of molecule;

Formula – string; molecular molecule;

 Molecular Weight – string; molecular weight;

 Status – string; status of availability;

 Type – string; type of availability;

 Largest Stock – string; maximum stock available in shop;

 Largest Stock Measure – string; measure;

 Largest Stock Measure Id – string; *MolPort* measure Id;

Synonyms – array of molecule names;

 Catalogues – array of :

Screening Block Suppliers – array of suppliers;

Building Block Suppliers – array of suppliers;

Virtual Suppliers – array of suppliers.

Method will return a Supplier objects with data structure:

Supplier Name – string; supplier name;

Supplier Id – int; supplier Id;

Minimum Order – double; minimum order for supplier;

Currency – string; currency ISO code;

Currency Id – int; *MolPort* currency identifier;

 Catalogues – array of supplier catalogues.

Method will return a Supplier objects with data structure:

Catalog Id – int; catalog Id in *MolPort* database;

Catalog Number – string; supplier catalog number;

 Stock – double; amount in stock;

 Stock Measure – string; amount measure;

 Stock Measure Id – int; amount measure Id in *MolPort* database;

 Last Update Date – string; last catalog update date in *MolPort* database;

Available Packings – array of packings.

Method will return a Packing objects with data structure:

Amount – string; amount;

 Measure – string; amount measure;

 Measure Id – int; amount measure Id in *MolPort* database;

 Price – double; price;

 Currency – string; currency;

 Currency Id – int; currency Id in *MolPort* database;

Delivery Days – int; days in which supplier sends out requested molecules if payment was made.

Method will return a Synonym objects with data structure:

Value – string; name/MDL number of molecule.

Record was not found:

|  |  |
| --- | --- |
| **Status** | **Response**  |
| 200 | { "Result": { "Status": 2, "Message": "Molecule was not found!" }, "Data": { "Version": "v.1.0" }} |

Record found:

|  |  |
| --- | --- |
| **Status** | **Response** |
| 200 | { "Result": { "Status": 1, "Message": "Molecule found!" }, "Data": { "Molecule": { "Id": 2325020, "MolPort Id": "MolPort-002-325-020", "SMILES": "CCOC(\u003dO)c1[nH]c2ccc(C)cc2c1NC(\u003dO)CC", "IUPAC": "ethyl 5-methyl-3-propanamido-1H-indole-2-carboxylate", "Formula": "C15H18N2O3", "Molecular Weight": 274.32, "Status": "shop", "Type": "stock", "Largest Stock": "124", "Largest Stock Measure": "mg", "Largest Stock Measure Id": 234, "Catalogues": { "Screening Block Suppliers": [ { "Supplier Name": "Specs", "Supplier Id": 2070, "Minimum Order": 200, "Currency": "USD", "Currency Id": 2, "Catalogues": [ { "Catalog Id": 84777984, "Catalog Number": "AG-690/10530016", "Stock": 2, "Stock Measure": "mg", "Stock Measure Id": 234, "Last Update Date": "today", "Available Packings": [ { "Amount": 2, "Measure": "mg", "Measure Id": 234, "Price": 32.20, "Currency": "USD", "Currency Id": 2, "Delivery Days": 7 } ] } ], "Shipment Costs": [ { "Price": 50, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "EUROPE", "Location Id": 1, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 50, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "USA", "Location Id": 2, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 50, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "CANADA AND MEXICO", "Location Id": 3, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 50, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "OTHER LOCATIONS", "Location Id": 4, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 } ] }, { "Supplier Name": "Vitas-M Laboratory, Ltd.", "Supplier Id": 2077, "Currency": "USD", "Currency Id": 2, "Catalogues": [ { "Catalog Id": 191573558, "Catalog Number": "STK374222", "Stock": 124, "Stock Measure": "mg", "Stock Measure Id": 234, "Purity": "\u003e90%", "Last Update Date": "this week", "Available Packings": [ { "Amount": 1, "Measure": "mg", "Measure Id": 234, "Price": 26.50, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 2, "Measure": "mg", "Measure Id": 234, "Price": 28.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 3, "Measure": "mg", "Measure Id": 234, "Price": 31.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 5, "Measure": "mg", "Measure Id": 234, "Price": 38.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 10, "Measure": "mg", "Measure Id": 234, "Price": 48.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 20, "Measure": "mg", "Measure Id": 234, "Price": 68.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 30, "Measure": "mg", "Measure Id": 234, "Price": 78.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 50, "Measure": "mg", "Measure Id": 234, "Price": 97.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 }, { "Amount": 100, "Measure": "mg", "Measure Id": 234, "Price": 161.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 10 } ] } ], "Shipment Costs": [ { "Price": 55, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "EUROPE", "Location Id": 1, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 55, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "USA", "Location Id": 2, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 55, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "CANADA AND MEXICO", "Location Id": 3, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 55, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "OTHER LOCATIONS", "Location Id": 4, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 } ] }, { "Supplier Name": "Princeton BioMolecular Research, Inc.", "Supplier Id": 2112, "Minimum Order": 150, "Currency": "USD", "Currency Id": 2, "Catalogues": [ { "Catalog Id": 208007160, "Catalog Number": "OSSL\_129598", "Stock Measure Id": 0, "Last Update Date": "last month", "Available Packings": [ { "Amount": 5, "Measure": "µmol", "Measure Id": 241, "Price": 19.85, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 10, "Measure": "µmol", "Measure Id": 241, "Price": 27.79, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 20, "Measure": "µmol", "Measure Id": 241, "Price": 31.76, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 1, "Measure": "mg", "Measure Id": 234, "Price": 15.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 2, "Measure": "mg", "Measure Id": 234, "Price": 17.64, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 3, "Measure": "mg", "Measure Id": 234, "Price": 19.85, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 5, "Measure": "mg", "Measure Id": 234, "Price": 23.82, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 7, "Measure": "mg", "Measure Id": 234, "Price": 27.79, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 10, "Measure": "mg", "Measure Id": 234, "Price": 31.76, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 15, "Measure": "mg", "Measure Id": 234, "Price": 35.73, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 20, "Measure": "mg", "Measure Id": 234, "Price": 39.70, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 25, "Measure": "mg", "Measure Id": 234, "Price": 49.50, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 30, "Measure": "mg", "Measure Id": 234, "Price": 54.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 35, "Measure": "mg", "Measure Id": 234, "Price": 58.50, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 40, "Measure": "mg", "Measure Id": 234, "Price": 65.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 50, "Measure": "mg", "Measure Id": 234, "Price": 80.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 }, { "Amount": 100, "Measure": "mg", "Measure Id": 234, "Price": 150.00, "Currency": "USD", "Currency Id": 2, "Delivery Days": 25 } ] } ], "Shipment Costs": [ { "Price": 110, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "EUROPE", "Location Id": 1, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 60, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "USA", "Location Id": 2, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 50, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "CANADA AND MEXICO", "Location Id": 3, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 }, { "Price": 120, "Currency": "USD", "Currency Id": 2, "Location Type": "REGION", "Location": "OTHER LOCATIONS", "Location Id": 4, "Shipment Type": "Basic Shipping", "Shipment Type Id": 3 } ] } ], "Building Block Suppliers": [], "Virtual Suppliers": [] }, "Synonyms": [ "ethyl", "ethyl 5-methyl-3-(propanoylamino)-1H-indole-2-carboxylate" ] }, "Version": "v.1.0" }} |

## 2. Search molecules with chemical search

Method to search molecules with chemical search if *SMILES* is known. Currently supported chemical search types are:

1. exact search;
2. exact fragment search;
3. similarity search;
4. perfect search;
5. substructure search;
6. superstructure search;

## Request

|  |  |
| --- | --- |
| **Method** | **URL**  |
| **GET** | /api/chemical-search/search |
| **JSON** | { "Structure":"CC(C)(C)OC(=O)N1CCCCCC1C(O)=O", "Search Type":4, "Filter Id":0, "Maximum Search Time":60000, "Maximum Result Count":1000, "Chemical Similarity Index":0.9}where: Structure – string; SMILES of molecule; Search Type – int, chemical search type with possible values: CHEMICAL\_SEARCH\_TYPE\_\_SUBSTRUCTURE = 1 CHEMICAL\_SEARCH\_TYPE\_\_SUPERSTRUCTURE = 2 CHEMICAL\_SEARCH\_TYPE\_\_EXACT = 3 CHEMICAL\_SEARCH\_TYPE\_\_SIMILARITY = 4 CHEMICAL\_SEARCH\_TYPE\_\_PERFECT = 5 CHEMICAL\_SEARCH\_TYPE\_\_EXACT\_FRAGMENT = 6 Maximum Search Time – int; time in miliseconds - maximum search time to be spent on chemical search; Maximum Result Count – int; maximum result count which must be returned as result; currently maximum allowed value is 1000; default value is 1000; Chemical Similarity Index – double; if similarity search is made, it is possible to provide similarity index in range 0 – 1; default value is 0.9. |

## Response

Method will return a list of Molecule objects with data structure:

{

"Id": <MolPort molecule id>,

"MolPort Id": <formatted MolPort molecule id>,

"SMILES": <SMILES>,

"Similarity Index": <Similarity index>

}

where:

Id – int; molecule identifier in *MolPort* database;

MolPort Id – string, formatted molecule identifier in *MolPort* database;

SMILES – string; *SMILES* of molecule;

Similarity Index – double; if similarity search was made, will contain similarity index

to initially searched molecule.

Molecules were not found:

|  |  |
| --- | --- |
| **Status** | **Response**  |
| 200 | { "Result": { "Status": 1, "Message": "Chemical search completed!" }, "Data": { "Molecules": [], "Version": "v.1.0" }} |

Molecules were found:

|  |  |
| --- | --- |
| **Status** | **Response**  |
| 200 | { "Result": { "Status": 2, "Message": "Index: 3, Size: 3" }, "Data": { "Molecules": [ { "Id": 160, "MolPort Id": "MolPort-000-000-160", "SMILES": "CNC(\u003dO)CCCN[C@@H](C)c1ccccc1 |r|" }, { "Id": 20665883, "MolPort Id": "MolPort-020-665-883", "SMILES": "CC(\u003dO)c1ccc(OCC(\u003dO)c2cn(CCC#N)c3ccccc23)cc1" }, { "Id": 28065133, "MolPort Id": "MolPort-028-065-133", "SMILES": "CC(NC(\u003dO)COc1ccc(cc1)C(C)\u003dO)c1cccs1" }, { "Id": 28065134, "MolPort Id": "MolPort-028-065-134" } ], "Version": "v.1.0" }} |